



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:52 PM UTC

PDB ID : 1N6F / pdb_00001n6f
Title : tricorn protease in complex with Z-Phe-diketo-Arg-Glu-Phe
Authors : Kim, J.-S.; Groll, M.; Huber, R.; Brandstetter, H.
Deposited on : 2002-11-10
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

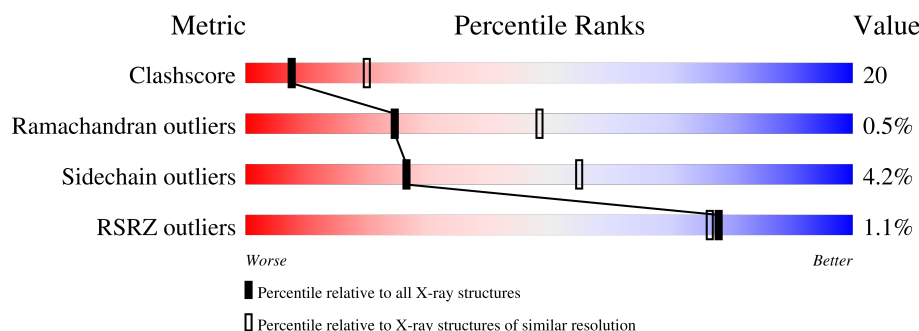
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	1071	2% 63% 29% . .
1	B	1071	% 62% 30% . .
1	C	1071	% 58% 34% . .
1	D	1071	% 60% 32% . .
1	E	1071	% 62% 30% . .
1	F	1071	% 59% 33% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

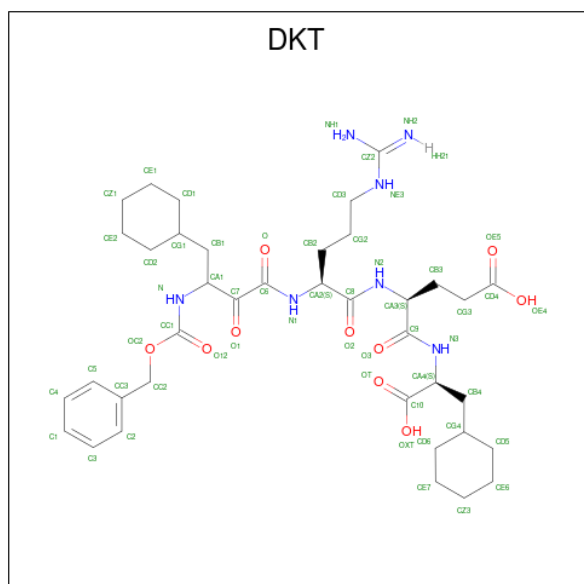
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DKT	A	1214	X	X	-	-
2	DKT	B	1214	X	X	-	-
2	DKT	C	1214	X	X	-	-
2	DKT	D	1214	X	X	-	-
2	DKT	E	1214	X	X	-	-
2	DKT	F	1214	X	X	-	-

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 tricorn protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1023	Total 8177	C 5196	N 1402	O 1551	S 28	94	0	0
1	B	1023	Total 8176	C 5196	N 1402	O 1550	S 28	94	0	0
1	C	1023	Total 8176	C 5196	N 1402	O 1550	S 28	94	0	0
1	D	1023	Total 8176	C 5196	N 1402	O 1550	S 28	94	0	0
1	E	1023	Total 8177	C 5196	N 1402	O 1551	S 28	94	0	0
1	F	1023	Total 8176	C 5196	N 1402	O 1550	S 28	94	0	0

- Molecule 2 is 4-[2-(3-BENZYLOXYCARBONYLAMINO-4-CYCLOHEXYL-1-HYDROXY-2-OXO-BUTYLAMINO)-5-GUANIDINO-PENTANOYLAMINO]-4-(1-CARBOXY-2-CYCLOHEXYL-ETHYLCARBAMOYL)-BUTYRIC ACID (CCD ID: DKT) (formula: $C_{38}H_{57}N_7O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			55	38	7	10		
2	B	1	Total	C	N	O	0	0
			55	38	7	10		
2	C	1	Total	C	N	O	0	0
			55	38	7	10		
2	D	1	Total	C	N	O	0	0
			55	38	7	10		
2	E	1	Total	C	N	O	0	0
			55	38	7	10		
2	F	1	Total	C	N	O	0	0
			55	38	7	10		

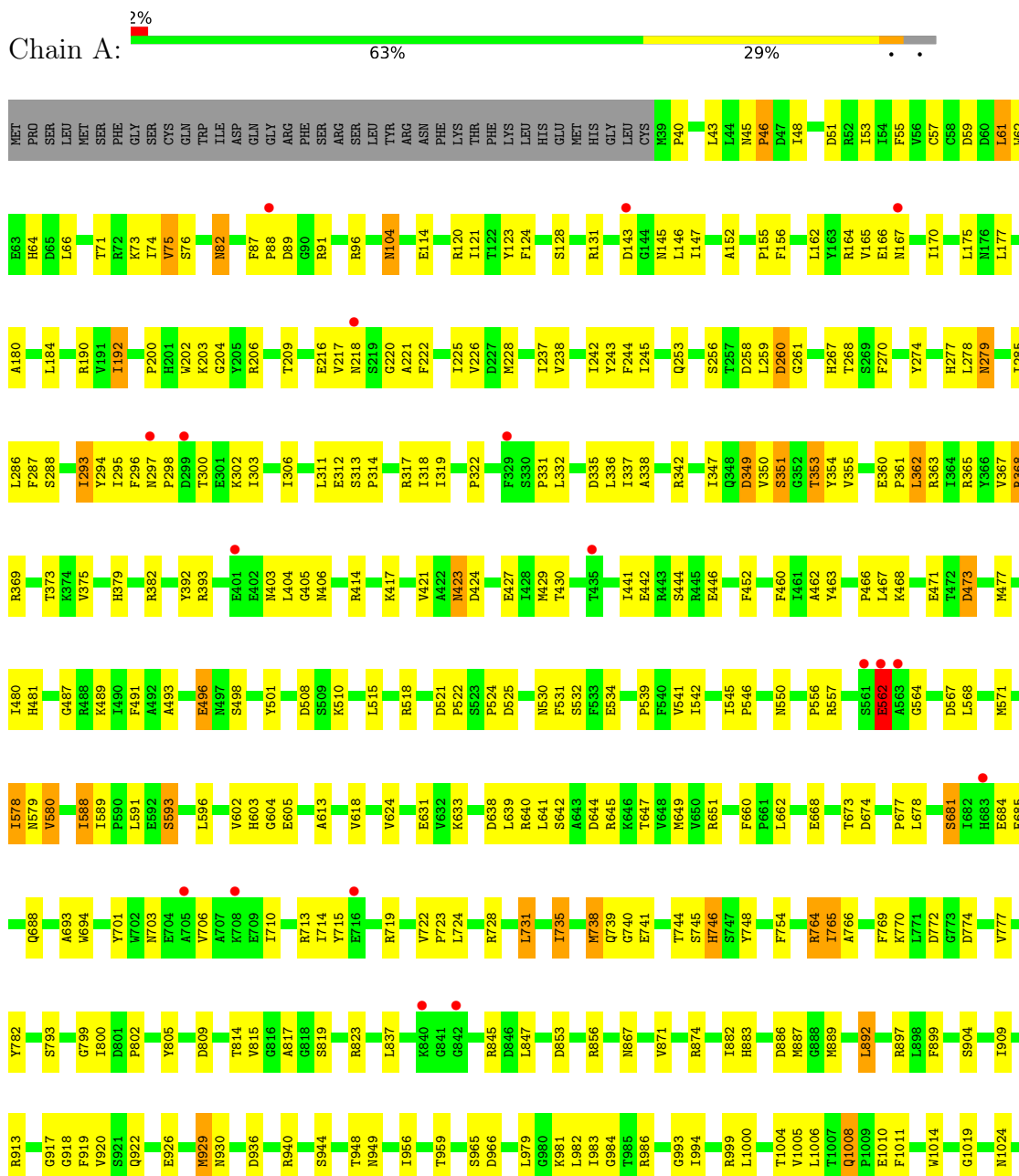
- Molecule 3 is water.

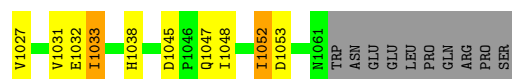
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	114	Total	O	0	0
			114	114		
3	B	108	Total	O	0	0
			108	108		
3	C	136	Total	O	0	0
			136	136		
3	D	132	Total	O	0	0
			132	132		
3	E	105	Total	O	0	0
			105	105		
3	F	104	Total	O	0	0
			104	104		

3 Residue-property plots

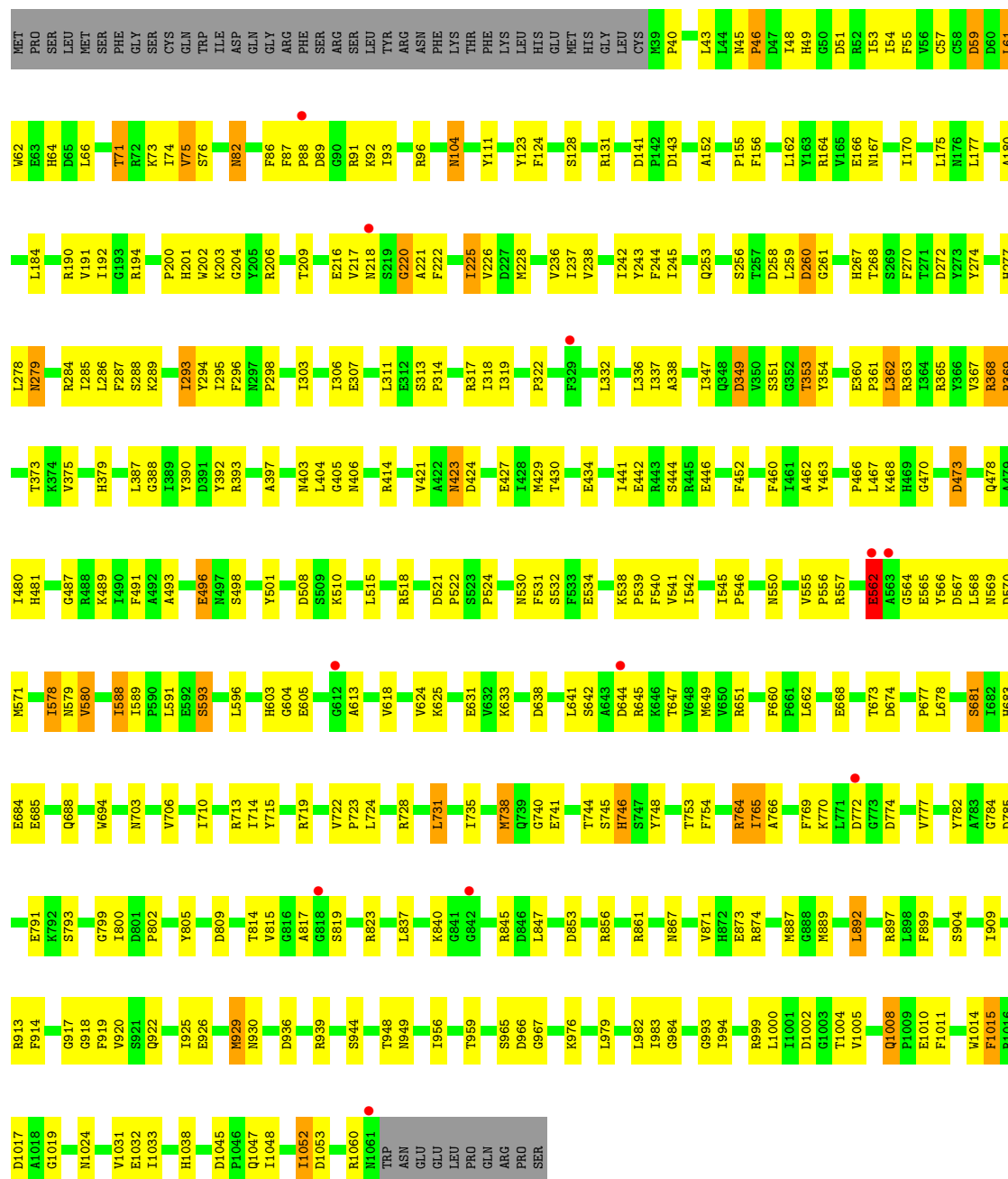
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: tricorn protease





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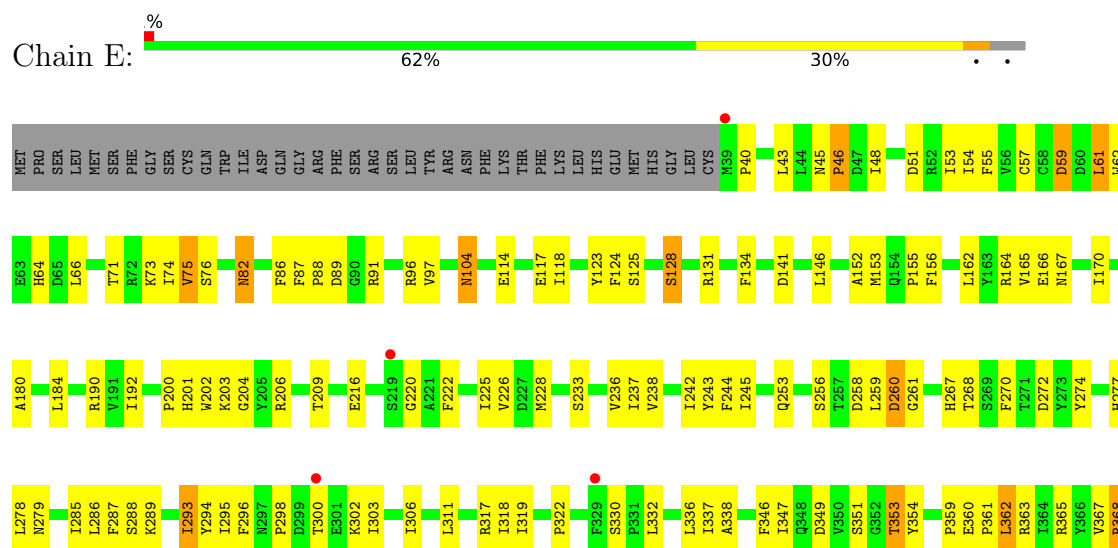
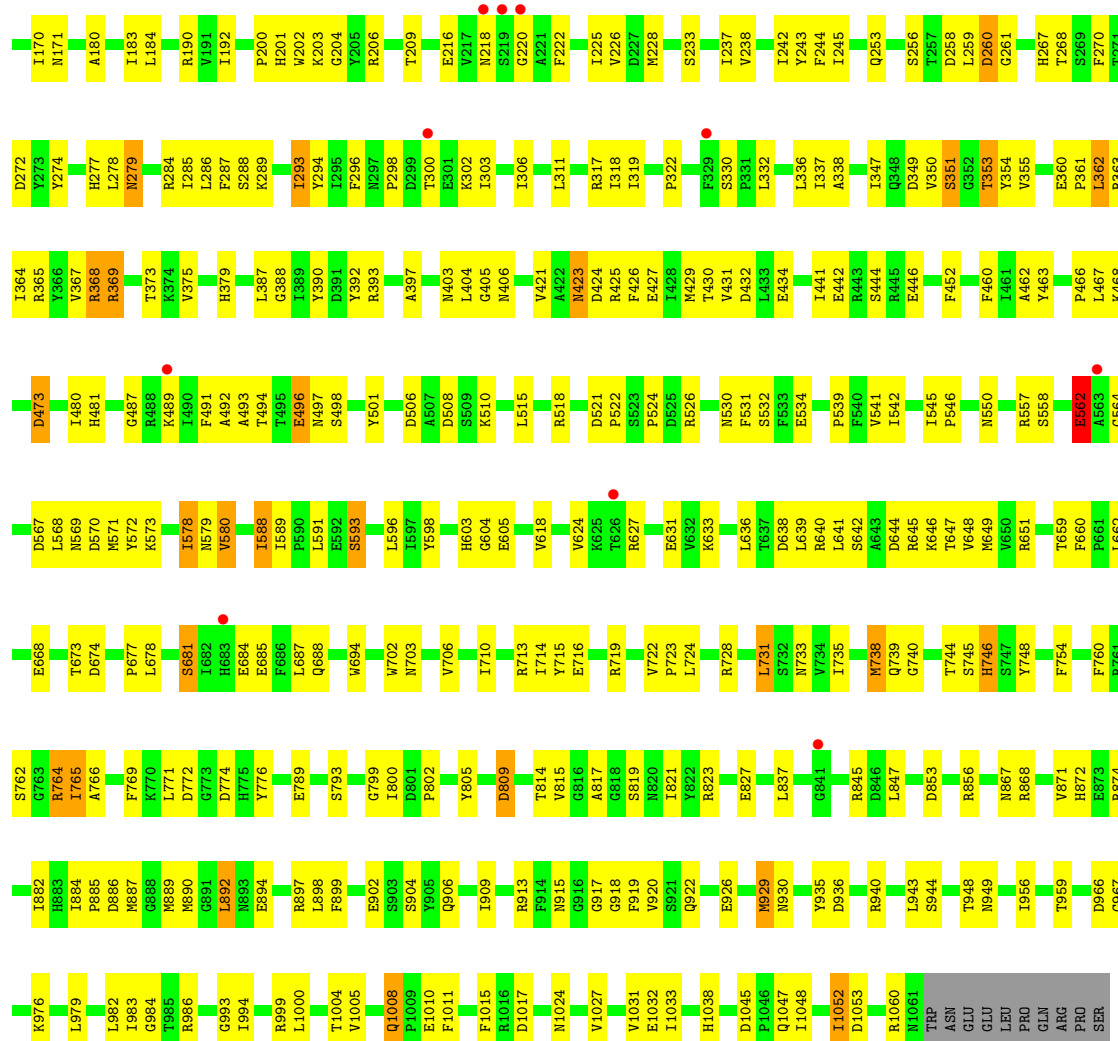


MET	PRO	SER	SER	LEU	MET	SER	PHE	GLY	SER	CYS	GLN	TRP	ILE	ASP	GLN	GLY	ARG	PHE	SER	SER	LEU	TYR	ASN	ASN	PHE	LYS	THR	PHE	LYS	LEU	HIS	GLU	MET	HIS	GLY	LEU	CYS	R39	P40	L43	L44	N45	P46	D47	I48	D51	R52	I53	I54	F55	V56	C57	C58	D59	D60	L61	W62
E63	H64	D65	L66	T71	R72	K73	I74	W75	S76	N82	R85	F86	P87	D88	G89	R90	R91	R96	V97	N98	R99	M104	Y109	E114	E117	I118	K119	R120	Y123	S125	S128	R131	D141	P142	D143	G144	N145	L146	A152	M153	Q154	P155	L166	N167													
L162	Y163	R164	V165	E166	N167	I170	V173	P174	L175	H176	L177	A180	T257	D258	L259	D260	G261	K262	D263	H267	T268	R269	F270	T271	L272	K273	L274	H277	N278	P279	L285	L286	F287	S288	K289	I293	Y294	L295	F296	N297	P298	E301	K302	I303	L306	E307	L311	P314	V322	R323	I317	I318	I319	P322	L332		
L336	I337	A338	F346	I347	Q348	D349	V350	L351	G352	T353	Y354	E360	L361	L362	R363	I364	R365	Y366	Y367	R368	R369	T373	V375	H379	F386	L387	G388	I389	Y390	D391	Y392	R393	A397	E401	E402	N403	L404	G405	N406	V421	A422	N423	D424	R317	I318	F426	E427	I428	M429	T430							
E434	V440	I441	E442	R443	S444	R445	E446	A447	M448	F452	F460	L461	A462	Y463	P466	L467	K468	D473	T480	H481	G487	R488	K489	L490	F491	A492	A493	E496	M497	S498	Y501	D508	S509	K510	L515	R518	D521	P522	S523	P524	N530	F531	S532	F533													
E534	V535	V536	Q537	K538	F540	V541	I542	I545	P546	N550	R557	S558	M559	E563	G564	D567	L568	M571	P577	I578	R579	V580	G583	I588	I589	P590	L591	E592	S593	L596	H603	G604	E605	A613	V618	V624	S622	E631	K633	D638																	
L641	S642	R645	Q646	T647	V648	M649	R651	T659	F660	P661	L662	E668	T673	D674	K675	P677	F678	V679	S680	S681	E684	E685	F686	L687	Q688	M689	Y690	W694	N703	V706	I710	R713	I714	Y715	R719	V722	P723	L724	R728	Y805	D809	T814	V815														
E737	M738	Q739	G740	E741	T744	S745	H746	S747	Y748	F754	F760	R761	G762	R764	I765	A766	C767	D768	F769	K770	L771	D772	G773	D774	H775	Y776	V777	V778	A779	K780	A781	Y782	Y786	S787	N788	E789	G790	E791	K792	S793	F796	G799	I800	D801	P802	G916	G917	G918	F919	V920	S921	Q922	E926				
Q816	A817	Q818	S819	R823	L837	R845	L846	L847	D853	R856	F857	I858	R861	N867	R868	R869	Y870	V871	R874	M887	K888	M889	M890	Q891	L892	N893	E894	L898	F899	S904	Y905	Q906	I909	V912	R913	F914	R915	G916	G917	G918	F919	V920	S921	Q922	E926												
M929	N930	D936	R939	R940	S944	T948	N949	G953	R954	I955	I956	T959	N960	G964	S965	D966	T969	F970	K975	K976	L977	G978	L979	L982	R983	G984	R985	R986	G993	I994	R999	L1000	T1004	V1005	Q1008	P1009	E1010	F1011	W1014	D1017	A1018	G1019															
M1024	V1027	D1028	V1031	E1032	I1033	H1038	D1045	F1046	Q1047	I1048	D1049	Y1050	A1051	I1052	D1053	N1061	TRP	ASN	GLU	GLU	LEU	PRO	GLN	ARG	PRO	PRO	SER																														

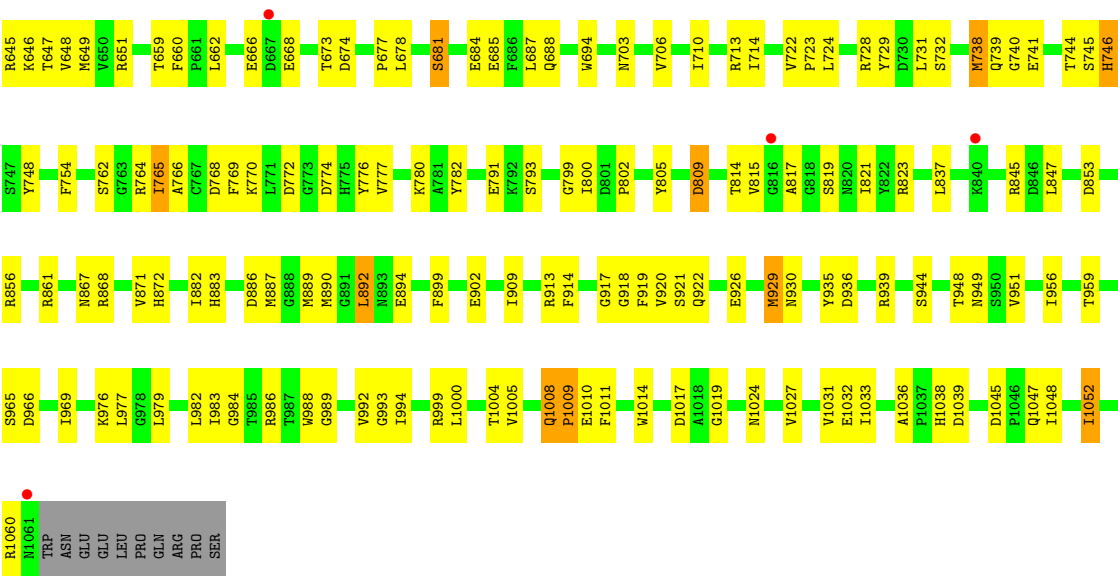
• Molecule 1: tricorn protease



MET	PRO	SER	LEU	MET	SER	PHE	GLY	SER	CYS	GLN	TRP	ILE	ASP	GLN	GLY	ARG	PHE	SER	SER	LEU	TYR	ASN	ASN	PHE	PHE	LYS	LEU	HIS	GLU	MET	HIS	GLY	LEU	CYS	R39	P40	L43	L44	N45	P46	D47	I48	D51	R52	I53	I54	F55	V56	C57	C58	D59	D60	L61	W62	
E63	H64	D65	L66	T71	R72	K73	I74	W75	S76	N82	R85	F87	P88	D89	G90	R91	R91	R96	V97	N98	R99	M104	Y105	Y109	E114	E117	I118	K119	R120	Y123	F124	S125	S128	T129	G130	R131	R131	A138	D141	A152	P155	L162	Y163	R164	V165	E166	N167								
L162	Y163	R164	V165	E166	N167	I170	V173	P174	L175	H176	L177	A180	T257	D258	L259	D260	G261	K262	D263	H267	T268	R269	F270	T271	L272	K273	L274	H277	N278	P279	L285	L286	F287	S288	K289	I293	Y294	L295	F296	N297	P298	E301	K302	I303	L306	E307	L311	P314	V322	R323	I317	I318	I319	P322	L332
L336	I337	A338	F346	I347	Q348	D349	V350	L351	G352	T353	Y354	E360	L361	L362	R363	I364	R365	Y366	Y367	R368	R369	T373	V375	H379	F386	L387	G388	I389	Y390	D391	Y392	R393	A397	E401	E402	N403	L404	G405	N406	V421	A422	N423	D424	R317	I318	F426	E427	I428	M429	T430					
E434	V440	I441	E442	R443	S444	R445	E446	A447	M448	F452	F460	L461	A462	Y463	P466	L467	K468	D473	T480	H481	G487	R488	K489	L490	F491	A492	A493	E496	M497	S498	Y501	D508	S509	K510	L515	R518	D521	P522	S523	P524	N530	F531	S532	F533											
E534	V535	V536	Q537	K538	F540	V541	I542	I545	P546	N550	R557	S558	M559	E563	G564	D567	L568	M571	P577	I578	R579	V580	G583	I588	I589	P590	L591	E592	S593	L596	H603	G604	E605	A613	V618	V624	S622	E631	K633	D638															
L641	S642	R645	Q646	T647	V648	M649	R651	T659	F660	P661	L662	E668	T673	D674	K675	P677	F678	V679	S680	S681	E684	E685	F686	L687	Q688	M689	Y690	W694	N703	V706	I710	R713	I714	Y715	R719	V722	P723	L724	R728	Y805	D809	T814	V815												
E737	M738	Q739	G740	E741	T744	S745	H746	S747	Y748	F754	F760	R761	G762	R764	I765	A766	C767	D768	F769	K770	L771	D772	G773	D774	H775	Y776	V777	V778	A779	K780	A781	Y782	Y786	S787	N788	E789	G790	E791	K792	S793	F796	G799	I800	D801	P802	G916	G917	G918	F919	V920	S921	Q922	E926		
Q816	A817	Q818	S819	R823	L837	R845	L846	L847	D853	R856	F857	I858	R861	N867	R868	R869	Y870	V871	R874	M887	K888	M889	M890	Q891	L892	N893	E894	L898	F899	S904	Y905	Q906	I909	V912	R913	F914	R915	G916	G917	G918	F919	V920	S921	Q922	E926										
M929	N930	D936	R939	R940	S944	T948	N949	G953	R954	I955	I956	T959	N960	G964	S965	D966	T969	F970	K975	K976	L977	G978	L979	L982	R983	G984	R985	R986	G993	I994	R999	L1000	T1004	V1005	Q1008	P1009	E1010	F1011	W1014	D1017	A1018	G1019													
M1024	V1027	D1028	V1031	E1032	I1033	H1038	D1045	F1046	Q1047	I1048	D1049	Y1050	A1051	I1052	D1053	N1061	TRP	ASN	GLU	GLU	LEU	PRO	GLN	ARG	PRO	PRO	SER																												







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.67Å 244.55Å 158.32Å 90.00° 104.59° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70 6.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	85.8 (6.00-2.70) 77.0 (6.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.71Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.280 0.247 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.52 , 74.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	50087	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	1/8367 (0.0%)	0.94	12/11311 (0.1%)
1	B	0.65	0/8366	0.94	13/11310 (0.1%)
1	C	0.61	1/8366 (0.0%)	0.94	11/11310 (0.1%)
1	D	0.62	0/8366	0.94	10/11310 (0.1%)
1	E	0.62	1/8367 (0.0%)	0.94	12/11311 (0.1%)
1	F	0.60	0/8366	0.94	13/11310 (0.1%)
All	All	0.62	3/50198 (0.0%)	0.94	71/67862 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	153	MET	SD-CE	5.36	1.93	1.79
1	E	153	MET	SD-CE	5.22	1.92	1.79
1	A	477	MET	SD-CE	-5.15	1.66	1.79

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	746	HIS	N-CA-C	6.87	120.97	111.90
1	B	1052	ILE	CB-CA-C	-6.78	103.34	111.81
1	C	1052	ILE	CB-CA-C	-6.76	103.36	111.81
1	E	1052	ILE	CB-CA-C	-6.59	103.57	111.81
1	D	746	HIS	N-CA-C	6.42	120.26	111.54
1	D	1052	ILE	CB-CA-C	-6.38	103.84	111.81
1	E	192	ILE	N-CA-C	6.27	116.90	107.75
1	F	1052	ILE	CB-CA-C	-6.23	104.02	111.81
1	A	1052	ILE	CB-CA-C	-6.17	104.10	111.81
1	E	746	HIS	N-CA-C	6.14	120.01	111.90
1	D	192	ILE	N-CA-C	6.02	116.54	108.11
1	C	746	HIS	N-CA-C	6.00	119.82	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	746	HIS	N-CA-C	5.90	119.69	111.90
1	F	746	HIS	N-CA-C	5.89	119.67	111.90
1	B	225	ILE	CB-CA-C	-5.76	105.01	110.65
1	D	362	LEU	N-CA-C	5.74	117.70	110.24
1	F	362	LEU	N-CA-C	5.74	117.70	110.24
1	A	192	ILE	N-CA-C	5.70	116.09	108.11
1	B	487	GLY	N-CA-C	-5.64	106.91	114.25
1	E	318	ILE	N-CA-C	5.64	117.46	108.89
1	B	192	ILE	N-CA-C	5.63	115.99	108.11
1	A	487	GLY	N-CA-C	-5.62	106.95	114.25
1	A	362	LEU	N-CA-C	5.62	117.54	110.24
1	F	487	GLY	N-CA-C	-5.61	106.96	114.25
1	A	782	TYR	N-CA-C	5.50	118.42	110.28
1	E	967	GLY	N-CA-C	-5.46	105.78	112.77
1	F	225	ILE	CB-CA-C	-5.44	104.75	110.62
1	D	318	ILE	N-CA-C	5.39	117.08	108.89
1	B	613	ALA	CA-C-N	5.38	125.28	119.85
1	B	613	ALA	C-N-CA	5.38	125.28	119.85
1	A	349	ASP	N-CA-C	-5.36	102.59	110.52
1	C	613	ALA	CA-C-N	5.35	125.25	119.85
1	C	613	ALA	C-N-CA	5.35	125.25	119.85
1	B	362	LEU	N-CA-C	5.33	117.17	110.24
1	D	1060	ARG	N-CA-C	-5.33	107.32	113.88
1	D	967	GLY	N-CA-C	-5.33	105.95	112.77
1	D	233	SER	N-CA-C	5.33	117.07	109.14
1	B	318	ILE	N-CA-C	5.29	116.94	108.89
1	C	487	GLY	N-CA-C	-5.29	107.38	114.25
1	E	1060	ARG	N-CA-C	-5.28	107.39	113.88
1	F	1060	ARG	N-CA-C	-5.27	107.40	113.88
1	A	318	ILE	N-CA-C	5.26	116.89	108.89
1	D	487	GLY	N-CA-C	-5.25	107.42	114.25
1	C	318	ILE	N-CA-C	5.24	116.92	108.85
1	E	904	SER	N-CA-C	5.24	118.49	112.57
1	A	735	ILE	N-CA-C	5.23	115.44	110.42
1	C	362	LEU	N-CA-C	5.23	117.03	110.24
1	E	233	SER	N-CA-C	5.23	116.93	109.14
1	F	782	TYR	N-CA-C	5.22	118.01	110.28
1	B	1060	ARG	N-CA-C	-5.22	107.46	113.88
1	B	349	ASP	N-CA-C	-5.21	103.51	110.55
1	B	782	TYR	N-CA-C	5.21	118.00	110.28
1	C	782	TYR	N-CA-C	5.21	117.99	110.28
1	F	192	ILE	N-CA-C	5.21	115.40	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	362	LEU	N-CA-C	5.19	116.99	110.24
1	F	349	ASP	N-CA-C	-5.19	103.55	110.55
1	E	487	GLY	N-CA-C	-5.19	107.36	114.67
1	C	192	ILE	N-CA-C	5.17	115.35	108.11
1	B	904	SER	N-CA-C	5.14	118.37	112.57
1	A	355	VAL	N-CA-C	5.12	115.34	108.17
1	C	679	VAL	N-CA-C	5.12	115.33	108.17
1	E	613	ALA	CA-C-N	5.10	125.00	119.85
1	E	613	ALA	C-N-CA	5.10	125.00	119.85
1	F	318	ILE	N-CA-C	5.10	116.70	108.85
1	F	355	VAL	N-CA-C	5.07	115.27	108.17
1	D	355	VAL	N-CA-C	5.07	115.21	108.11
1	F	78	LEU	N-CA-C	-5.07	107.13	113.72
1	A	613	ALA	CA-C-N	5.05	124.95	119.85
1	A	613	ALA	C-N-CA	5.05	124.95	119.85
1	F	969	ILE	CB-CA-C	-5.05	105.42	111.88
1	C	233	SER	N-CA-C	5.04	116.65	109.14

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	8177	0	8003	310	0
1	B	8176	0	8000	307	0
1	C	8176	0	8000	399	0
1	D	8176	0	8000	332	0
1	E	8177	0	8003	316	0
1	F	8176	0	8000	371	0
2	A	55	0	46	20	0
2	B	55	0	46	7	0
2	C	55	0	46	8	0
2	D	55	0	46	8	0
2	E	55	0	46	18	0
2	F	55	0	46	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	114	0	0	36	0
3	B	108	0	0	38	0
3	C	136	0	0	94	0
3	D	132	0	0	54	0
3	E	105	0	0	24	0
3	F	104	0	0	87	0
All	All	50087	0	48282	1943	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 20.

All (1943) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:SER:HB3	2:A:1214:DKT:C7	1.23	1.62
1:F:965:SER:CB	2:F:1214:DKT:O1	1.64	1.46
1:A:965:SER:CB	2:A:1214:DKT:O1	1.63	1.46
1:E:965:SER:CB	2:E:1214:DKT:O1	1.64	1.43
1:E:965:SER:CB	2:E:1214:DKT:C7	2.02	1.38
1:F:965:SER:CB	2:F:1214:DKT:C7	2.02	1.37
1:E:965:SER:HB3	2:E:1214:DKT:C7	1.52	1.36
1:D:171:ASN:HB3	3:D:1215:HOH:O	1.25	1.28
1:A:965:SER:CB	2:A:1214:DKT:C7	2.03	1.27
1:E:965:SER:OG	2:E:1214:DKT:C7	1.87	1.20
1:F:476:VAL:HG13	3:F:1283:HOH:O	1.41	1.20
2:A:1214:DKT:HE61	3:A:1276:HOH:O	1.51	1.08
1:F:97:VAL:HG12	3:F:1217:HOH:O	1.55	1.06
3:C:1231:HOH:O	1:D:702:TRP:HA	1.53	1.06
1:C:741:GLU:HB3	3:C:1322:HOH:O	1.54	1.05
1:A:966:ASP:N	2:A:1214:DKT:O1	1.90	1.05
1:C:771:LEU:HD22	3:C:1234:HOH:O	1.56	1.05
1:A:143:ASP:HA	3:A:1291:HOH:O	1.57	1.04
1:E:966:ASP:N	2:E:1214:DKT:O1	1.90	1.03
1:F:966:ASP:N	2:F:1214:DKT:O1	1.91	1.03
1:B:220:GLY:HA2	3:B:1278:HOH:O	1.60	1.02
1:E:965:SER:HB3	2:E:1214:DKT:C6	1.89	1.02
1:E:965:SER:HB3	2:E:1214:DKT:O1	0.82	0.98
1:D:966:ASP:N	2:D:1214:DKT:O1	1.90	0.97
1:E:965:SER:CB	2:E:1214:DKT:C6	2.43	0.96
1:A:965:SER:HB3	2:A:1214:DKT:C6	1.94	0.96
1:A:192:ILE:HG13	3:A:1266:HOH:O	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:966:ASP:N	2:B:1214:DKT:O1	1.92	0.95
1:A:965:SER:CB	2:A:1214:DKT:C6	2.45	0.94
1:F:965:SER:CB	2:F:1214:DKT:C6	2.44	0.94
1:C:124:PHE:HB2	3:C:1232:HOH:O	1.68	0.93
1:B:625:LYS:HG3	3:B:1268:HOH:O	1.69	0.92
1:F:173:VAL:HB	3:F:1250:HOH:O	1.69	0.91
1:B:1015:PHE:HB3	3:B:1283:HOH:O	1.71	0.91
1:E:948:THR:H	1:F:922:GLN:HE22	1.17	0.90
1:A:297:ASN:HB2	3:A:1319:HOH:O	1.70	0.90
1:C:446:GLU:N	3:C:1263:HOH:O	2.03	0.90
1:D:494:THR:HA	3:D:1240:HOH:O	1.71	0.90
1:C:82:ASN:HA	3:C:1216:HOH:O	1.71	0.89
1:C:966:ASP:N	2:C:1214:DKT:O1	1.93	0.89
1:A:965:SER:HB3	2:A:1214:DKT:O1	0.71	0.89
1:C:557:ARG:HH22	1:C:562:GLU:H	1.23	0.87
1:D:557:ARG:HH22	1:D:562:GLU:H	1.23	0.86
1:D:99:ARG:HB2	3:D:1297:HOH:O	1.75	0.86
1:F:557:ARG:HH22	1:F:562:GLU:H	1.22	0.86
1:A:525:ASP:HA	3:B:1262:HOH:O	1.75	0.85
1:E:557:ARG:HH22	1:E:562:GLU:H	1.24	0.85
1:A:557:ARG:HH22	1:A:562:GLU:H	1.23	0.85
1:B:206:ARG:H	1:B:1024:ASN:HD21	1.24	0.84
1:C:245:ILE:HB	3:C:1223:HOH:O	1.78	0.83
1:A:253:GLN:HE22	1:A:270:PHE:H	1.27	0.83
1:F:164:ARG:HB3	3:F:1250:HOH:O	1.78	0.83
1:C:401:GLU:HB2	3:C:1243:HOH:O	1.79	0.83
1:F:206:ARG:H	1:F:1024:ASN:HD21	1.25	0.83
1:A:40:PRO:HG2	1:A:724:LEU:HD22	1.62	0.82
1:D:760:PHE:HD2	3:D:1297:HOH:O	1.61	0.82
1:C:206:ARG:H	1:C:1024:ASN:HD21	1.27	0.82
1:B:784:GLY:HA3	3:B:1236:HOH:O	1.78	0.82
1:F:253:GLN:HE22	1:F:270:PHE:H	1.26	0.82
1:F:526:ARG:HD3	3:F:1225:HOH:O	1.80	0.82
1:B:557:ARG:HH22	1:B:562:GLU:H	1.22	0.81
1:E:134:PHE:HB2	3:E:1286:HOH:O	1.80	0.81
1:A:948:THR:H	1:B:922:GLN:HE22	1.29	0.81
1:E:253:GLN:HE22	1:E:270:PHE:H	1.27	0.81
1:E:922:GLN:HE22	1:F:948:THR:H	1.25	0.81
1:C:253:GLN:HE22	1:C:270:PHE:H	1.26	0.81
1:B:317:ARG:HD3	1:E:823:ARG:HD2	1.60	0.81
1:D:253:GLN:HE22	1:D:270:PHE:H	1.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:775:HIS:O	3:C:1234:HOH:O	1.98	0.81
1:A:206:ARG:H	1:A:1024:ASN:ND2	1.80	0.80
1:D:871:VAL:HG22	1:D:1052:ILE:HD11	1.62	0.80
1:A:317:ARG:HD3	1:D:823:ARG:HD2	1.63	0.80
1:B:143:ASP:HA	3:B:1287:HOH:O	1.80	0.80
1:C:337:ILE:HD12	1:C:649:MET:CE	2.12	0.80
1:B:871:VAL:HG22	1:B:1052:ILE:HD11	1.64	0.80
1:F:1036:ALA:HB3	3:F:1267:HOH:O	1.80	0.79
1:B:40:PRO:HG2	1:B:724:LEU:HD22	1.62	0.79
1:B:284:ARG:HD3	3:B:1222:HOH:O	1.82	0.79
1:B:295:ILE:HD13	3:B:1320:HOH:O	1.81	0.79
1:E:40:PRO:HG2	1:E:724:LEU:HD22	1.65	0.79
1:A:206:ARG:H	1:A:1024:ASN:HD21	1.26	0.79
1:B:253:GLN:HE22	1:B:270:PHE:H	1.31	0.79
1:D:206:ARG:H	1:D:1024:ASN:HD21	1.29	0.79
1:A:897:ARG:NE	3:A:1217:HOH:O	2.15	0.79
1:C:173:VAL:HB	3:C:1219:HOH:O	1.82	0.79
1:F:992:VAL:HB	3:F:1257:HOH:O	1.81	0.79
1:C:403:ASN:ND2	1:C:405:GLY:H	1.81	0.78
1:F:337:ILE:HD12	1:F:649:MET:CE	2.12	0.78
1:F:918:GLY:N	2:F:1214:DKT:O	2.16	0.78
1:B:337:ILE:HD12	1:B:649:MET:CE	2.12	0.78
1:C:871:VAL:HG22	1:C:1052:ILE:HD11	1.64	0.78
1:D:636:LEU:HB3	3:D:1310:HOH:O	1.82	0.78
1:A:815:VAL:HA	1:A:819:SER:HB3	1.64	0.78
1:B:918:GLY:N	2:B:1214:DKT:O	2.16	0.78
1:C:40:PRO:HG2	1:C:724:LEU:HD22	1.66	0.78
1:D:530:ASN:ND2	1:D:531:PHE:H	1.82	0.78
1:D:918:GLY:N	2:D:1214:DKT:O	2.16	0.78
1:F:815:VAL:HA	1:F:819:SER:HB3	1.65	0.78
1:E:206:ARG:H	1:E:1024:ASN:HD21	1.31	0.78
1:D:218:ASN:HB2	3:D:1258:HOH:O	1.84	0.78
1:E:337:ILE:HD12	1:E:649:MET:CE	2.14	0.78
1:D:349:ASP:OD2	1:D:351:SER:HB3	1.84	0.78
1:E:88:PRO:HB3	3:E:1234:HOH:O	1.81	0.78
1:F:871:VAL:HG22	1:F:1052:ILE:HD11	1.64	0.77
1:A:871:VAL:HG22	1:A:1052:ILE:HD11	1.65	0.77
1:B:421:VAL:HB	1:B:429:MET:HE3	1.64	0.77
1:F:203:LYS:HA	3:F:1226:HOH:O	1.84	0.77
1:E:349:ASP:OD2	1:E:351:SER:HB3	1.84	0.77
1:B:206:ARG:H	1:B:1024:ASN:ND2	1.81	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:GLY:N	2:A:1214:DKT:O	2.18	0.77
1:C:263:ASP:HB2	3:C:1284:HOH:O	1.83	0.77
1:F:40:PRO:HG2	1:F:724:LEU:HD22	1.65	0.77
1:E:530:ASN:ND2	1:E:531:PHE:H	1.82	0.77
1:B:268:THR:HG22	1:B:303:ILE:HD11	1.66	0.77
1:C:922:GLN:HE22	1:D:948:THR:H	1.29	0.77
1:E:918:GLY:N	2:E:1214:DKT:O	2.18	0.77
1:A:403:ASN:ND2	1:A:405:GLY:H	1.83	0.77
1:B:815:VAL:HA	1:B:819:SER:HB3	1.67	0.77
1:A:73:LYS:HD3	1:A:76:SER:HB3	1.68	0.76
1:A:337:ILE:HD12	1:A:649:MET:CE	2.15	0.76
1:A:53:ILE:HG23	1:A:286:LEU:HD21	1.67	0.76
1:E:403:ASN:ND2	1:E:405:GLY:H	1.83	0.76
1:E:518:ARG:NH1	3:E:1278:HOH:O	2.19	0.76
1:C:970:PHE:HA	3:C:1252:HOH:O	1.83	0.76
1:B:73:LYS:HD3	1:B:76:SER:HB3	1.67	0.76
1:C:918:GLY:N	2:C:1214:DKT:O	2.18	0.76
1:D:268:THR:HG22	1:D:303:ILE:HD11	1.66	0.76
1:E:871:VAL:HG22	1:E:1052:ILE:HD11	1.65	0.76
1:D:337:ILE:HD12	1:D:649:MET:CE	2.14	0.76
1:B:87:PHE:HB3	1:B:88:PRO:HD2	1.68	0.76
1:E:568:LEU:HB3	1:E:571:MET:HE2	1.66	0.76
1:C:948:THR:H	1:D:922:GLN:HE22	1.33	0.76
1:A:530:ASN:ND2	1:A:531:PHE:H	1.84	0.75
1:E:53:ILE:HG23	1:E:286:LEU:HD21	1.66	0.75
1:D:40:PRO:HG2	1:D:724:LEU:HD22	1.65	0.75
1:A:596:LEU:HD11	1:A:662:LEU:HD11	1.68	0.75
1:D:815:VAL:HA	1:D:819:SER:HB3	1.67	0.75
1:E:578:ILE:HD11	1:E:580:VAL:HG23	1.68	0.75
1:F:403:ASN:ND2	1:F:405:GLY:H	1.83	0.75
1:F:939:ARG:NH2	3:F:1216:HOH:O	2.20	0.75
1:E:268:THR:HG22	1:E:303:ILE:HD11	1.69	0.75
1:D:53:ILE:HG23	1:D:286:LEU:HD21	1.69	0.75
1:E:421:VAL:HB	1:E:429:MET:HE3	1.69	0.75
1:C:206:ARG:H	1:C:1024:ASN:ND2	1.83	0.75
1:D:578:ILE:HD11	1:D:580:VAL:HG23	1.69	0.75
1:E:815:VAL:HA	1:E:819:SER:HB3	1.69	0.75
1:F:162:LEU:HD22	3:F:1293:HOH:O	1.86	0.75
1:C:578:ILE:HD11	1:C:580:VAL:HG23	1.68	0.74
1:D:351:SER:OG	1:D:353:THR:HG22	1.87	0.74
1:F:206:ARG:H	1:F:1024:ASN:ND2	1.83	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:979:LEU:HB3	3:C:1316:HOH:O	1.85	0.74
1:D:760:PHE:CD2	3:D:1297:HOH:O	2.36	0.74
1:F:73:LYS:HD3	1:F:76:SER:HB3	1.68	0.74
1:D:403:ASN:ND2	1:D:405:GLY:H	1.84	0.74
1:B:337:ILE:HD12	1:B:649:MET:HE1	1.70	0.74
1:B:578:ILE:HD11	1:B:580:VAL:HG23	1.70	0.74
1:C:815:VAL:HA	1:C:819:SER:HB3	1.66	0.74
1:C:955:ILE:HD12	3:C:1316:HOH:O	1.86	0.74
1:D:206:ARG:H	1:D:1024:ASN:ND2	1.84	0.74
1:D:260:ASP:OD1	3:D:1326:HOH:O	2.05	0.74
1:E:351:SER:OG	1:E:353:THR:HG22	1.88	0.74
1:F:596:LEU:HD11	1:F:662:LEU:HD11	1.68	0.74
1:C:994:ILE:HG22	1:C:1008:GLN:O	1.87	0.74
1:A:268:THR:HG22	1:A:303:ILE:HD11	1.69	0.74
1:C:796:PHE:HA	3:C:1269:HOH:O	1.87	0.74
1:F:53:ILE:HG23	1:F:286:LEU:HD21	1.70	0.74
1:A:965:SER:OG	2:A:1214:DKT:C7	2.36	0.73
1:C:366:TYR:HB3	3:C:1251:HOH:O	1.89	0.73
1:D:596:LEU:HD11	1:D:662:LEU:HD11	1.70	0.73
1:E:167:ASN:HB2	1:E:170:ILE:HB	1.70	0.73
1:D:403:ASN:HD22	1:D:404:LEU:N	1.86	0.73
1:C:823:ARG:HD2	1:F:317:ARG:HD3	1.70	0.73
1:F:167:ASN:HB2	1:F:170:ILE:HB	1.69	0.73
1:F:337:ILE:HD12	1:F:649:MET:HE1	1.70	0.73
1:F:355:VAL:HG13	3:F:1299:HOH:O	1.88	0.73
1:D:421:VAL:HB	1:D:429:MET:HE3	1.69	0.73
1:C:351:SER:OG	1:C:353:THR:HG22	1.88	0.73
1:A:421:VAL:HB	1:A:429:MET:HE3	1.70	0.73
1:B:873:GLU:OE2	3:B:1244:HOH:O	2.07	0.73
1:C:268:THR:HG22	1:C:303:ILE:HD11	1.71	0.72
2:C:1214:DKT:HB12	3:C:1276:HOH:O	1.86	0.72
1:E:87:PHE:HB3	1:E:88:PRO:HD2	1.70	0.72
1:E:337:ILE:HD12	1:E:649:MET:HE1	1.71	0.72
1:E:596:LEU:HD11	1:E:662:LEU:HD11	1.71	0.72
1:C:167:ASN:HB2	1:C:170:ILE:HB	1.72	0.72
1:F:578:ILE:HD11	1:F:580:VAL:HG23	1.69	0.72
1:C:403:ASN:HD22	1:C:404:LEU:N	1.87	0.72
1:B:349:ASP:OD2	1:B:351:SER:HB3	1.89	0.72
1:C:349:ASP:OD2	1:C:351:SER:HB3	1.88	0.72
1:C:164:ARG:HB3	3:C:1219:HOH:O	1.90	0.72
1:D:73:LYS:HD3	1:D:76:SER:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:ARG:H	1:E:1024:ASN:ND2	1.86	0.72
1:A:922:GLN:HE22	1:B:948:THR:H	1.37	0.72
1:B:351:SER:OG	1:B:353:THR:HG22	1.89	0.71
1:C:393:ARG:CZ	1:E:558:SER:HA	2.20	0.71
1:F:349:ASP:OD2	1:F:351:SER:HB3	1.89	0.71
1:C:53:ILE:HG23	1:C:286:LEU:HD21	1.72	0.71
1:E:948:THR:H	1:F:922:GLN:NE2	1.86	0.71
1:A:351:SER:OG	1:A:353:THR:HG22	1.90	0.71
1:C:530:ASN:ND2	1:C:531:PHE:H	1.88	0.71
1:A:578:ILE:HD11	1:A:580:VAL:HG23	1.72	0.71
1:C:596:LEU:HD11	1:C:662:LEU:HD11	1.72	0.71
1:B:53:ILE:HG23	1:B:286:LEU:HD21	1.72	0.71
1:C:421:VAL:HB	1:C:429:MET:HE3	1.72	0.71
1:C:430:THR:C	3:C:1227:HOH:O	2.34	0.71
1:D:568:LEU:HB3	1:D:571:MET:HE2	1.70	0.71
1:D:994:ILE:HG22	1:D:1008:GLN:O	1.91	0.71
1:A:746:HIS:NE2	1:A:965:SER:OG	2.24	0.71
1:B:403:ASN:ND2	1:B:405:GLY:H	1.87	0.71
1:E:922:GLN:NE2	1:F:948:THR:H	1.89	0.71
1:E:403:ASN:HD22	1:E:404:LEU:N	1.88	0.71
1:C:191:VAL:HG23	3:C:1215:HOH:O	1.91	0.71
1:D:332:LEU:HD11	1:D:338:ALA:HB2	1.72	0.71
1:D:571:MET:HB3	3:D:1256:HOH:O	1.89	0.71
1:F:530:ASN:ND2	1:F:531:PHE:H	1.89	0.71
1:A:104:ASN:HB2	3:A:1271:HOH:O	1.91	0.71
1:A:403:ASN:HD22	1:A:404:LEU:N	1.89	0.71
1:B:596:LEU:HD11	1:B:662:LEU:HD11	1.72	0.71
1:C:203:LYS:NZ	3:C:1237:HOH:O	2.23	0.71
1:C:73:LYS:HD3	1:C:76:SER:HB3	1.72	0.70
1:A:61:LEU:HB3	1:A:75:VAL:HG13	1.73	0.70
1:B:61:LEU:HB3	1:B:75:VAL:HG13	1.71	0.70
1:D:167:ASN:HB2	1:D:170:ILE:HB	1.72	0.70
1:A:167:ASN:HB2	1:A:170:ILE:HB	1.73	0.70
1:C:222:PHE:N	3:C:1327:HOH:O	2.25	0.70
1:D:468:LYS:HD2	1:D:473:ASP:HB3	1.73	0.70
1:F:468:LYS:HD2	1:F:473:ASP:HB3	1.72	0.70
1:F:1024:ASN:HA	3:F:1244:HOH:O	1.90	0.70
1:D:935:TYR:HB3	3:D:1269:HOH:O	1.89	0.70
1:A:568:LEU:HB3	1:A:571:MET:HE2	1.71	0.70
1:E:73:LYS:HD3	1:E:76:SER:HB3	1.72	0.70
1:E:994:ILE:HG22	1:E:1008:GLN:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:PHE:HB3	1:C:88:PRO:HD2	1.74	0.70
1:B:994:ILE:HG22	1:B:1008:GLN:O	1.92	0.69
1:C:337:ILE:HD12	1:C:649:MET:HE1	1.72	0.69
1:D:337:ILE:HD12	1:D:649:MET:HE1	1.72	0.69
1:F:87:PHE:HB3	1:F:88:PRO:HD2	1.74	0.69
2:D:1214:DKT:OT	3:D:1282:HOH:O	2.10	0.69
1:E:61:LEU:HB3	1:E:75:VAL:HG13	1.74	0.69
1:F:421:VAL:HB	1:F:429:MET:HE3	1.72	0.69
1:C:82:ASN:H	1:C:82:ASN:HD22	1.38	0.69
1:F:153:MET:HB3	3:F:1294:HOH:O	1.91	0.69
1:F:403:ASN:HD22	1:F:404:LEU:N	1.90	0.69
1:C:317:ARG:HD3	1:F:823:ARG:HD2	1.73	0.69
1:D:61:LEU:HD13	1:D:74:ILE:HD11	1.74	0.69
1:F:51:ASP:O	3:F:1222:HOH:O	2.09	0.69
1:F:332:LEU:HD11	1:F:338:ALA:HB2	1.74	0.69
1:F:994:ILE:HG22	1:F:1008:GLN:O	1.92	0.69
1:F:268:THR:HG22	1:F:303:ILE:HD11	1.73	0.69
1:C:307:GLU:HG2	3:C:1304:HOH:O	1.92	0.69
1:D:446:GLU:OE1	1:D:468:LYS:HE2	1.93	0.69
1:E:322:PRO:HA	1:E:678:LEU:HD22	1.75	0.69
1:C:678:LEU:HG	3:C:1291:HOH:O	1.92	0.69
1:D:87:PHE:HB3	1:D:88:PRO:HD2	1.73	0.69
1:D:432:ASP:N	3:D:1262:HOH:O	2.26	0.69
1:D:530:ASN:HD22	1:D:531:PHE:H	1.41	0.69
1:A:87:PHE:HB3	1:A:88:PRO:HD2	1.75	0.69
1:A:994:ILE:HG22	1:A:1008:GLN:O	1.94	0.68
1:C:368:ARG:NH2	3:C:1251:HOH:O	2.25	0.68
1:D:322:PRO:HA	1:D:678:LEU:HD22	1.75	0.68
1:F:603:HIS:NE2	3:F:1235:HOH:O	2.25	0.68
1:C:279:ASN:ND2	3:C:1245:HOH:O	2.06	0.68
1:A:61:LEU:HD13	1:A:74:ILE:HD11	1.75	0.68
1:B:403:ASN:HD22	1:B:404:LEU:N	1.92	0.68
1:C:737:GLU:HA	3:C:1237:HOH:O	1.92	0.68
1:E:332:LEU:HD11	1:E:338:ALA:HB2	1.74	0.68
1:E:530:ASN:HD22	1:E:531:PHE:H	1.40	0.68
1:A:167:ASN:HB3	3:A:1301:HOH:O	1.93	0.68
1:B:322:PRO:HA	1:B:678:LEU:HD22	1.75	0.68
1:E:486:GLU:HB2	3:E:1231:HOH:O	1.93	0.68
1:A:349:ASP:OD2	1:A:351:SER:HB3	1.94	0.68
1:E:468:LYS:HD2	1:E:473:ASP:HB3	1.75	0.68
1:E:61:LEU:HD13	1:E:74:ILE:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:939:ARG:N	3:C:1231:HOH:O	2.27	0.68
1:D:982:LEU:C	1:D:983:ILE:HD12	2.19	0.68
1:C:332:LEU:HD11	1:C:338:ALA:HB2	1.76	0.68
1:C:766:ALA:HB3	1:C:793:SER:HA	1.76	0.68
1:C:1027:VAL:HA	3:C:1217:HOH:O	1.94	0.68
1:D:929:MET:HE3	1:D:979:LEU:HD11	1.76	0.68
1:A:948:THR:H	1:B:922:GLN:NE2	1.91	0.67
1:B:530:ASN:ND2	1:B:531:PHE:H	1.92	0.67
1:C:446:GLU:OE1	1:C:468:LYS:HE2	1.94	0.67
1:D:190:ARG:HG3	1:D:216:GLU:OE2	1.93	0.67
1:F:322:PRO:HA	1:F:678:LEU:HD22	1.76	0.67
1:B:468:LYS:HD2	1:B:473:ASP:HB3	1.77	0.67
1:B:568:LEU:HB3	1:B:571:MET:HE2	1.74	0.67
1:F:913:ARG:HH21	1:F:1047:GLN:HE21	1.41	0.67
1:C:61:LEU:HB3	1:C:75:VAL:HG13	1.74	0.67
1:C:123:TYR:OH	1:C:823:ARG:HD3	1.95	0.67
1:D:558:SER:HA	1:F:393:ARG:CZ	2.24	0.67
1:F:568:LEU:HB3	1:F:571:MET:HE2	1.76	0.67
1:A:206:ARG:N	1:A:1024:ASN:HD21	1.93	0.67
1:D:403:ASN:HD22	1:D:403:ASN:C	2.03	0.67
1:B:167:ASN:HB2	1:B:170:ILE:HB	1.75	0.67
1:C:403:ASN:HD22	1:C:403:ASN:C	2.02	0.67
1:E:499:HIS:HD2	3:E:1221:HOH:O	1.77	0.67
1:D:913:ARG:HH21	1:D:1047:GLN:HE21	1.41	0.67
1:F:61:LEU:HB3	1:F:75:VAL:HG13	1.75	0.67
1:F:403:ASN:HD22	1:F:403:ASN:C	2.02	0.67
1:C:164:ARG:O	3:C:1219:HOH:O	2.12	0.66
1:C:724:LEU:O	3:C:1289:HOH:O	2.13	0.66
1:C:929:MET:HE3	1:C:979:LEU:HD11	1.76	0.66
1:D:639:LEU:HG	3:D:1218:HOH:O	1.95	0.66
1:E:190:ARG:HG3	1:E:216:GLU:OE2	1.95	0.66
1:A:337:ILE:HD12	1:A:649:MET:HE1	1.75	0.66
1:A:530:ASN:HD22	1:A:531:PHE:H	1.42	0.66
1:C:322:PRO:HA	1:C:678:LEU:HD22	1.77	0.66
1:D:897:ARG:NE	3:D:1267:HOH:O	2.28	0.66
1:F:65:ASP:OD1	3:F:1222:HOH:O	2.13	0.66
1:F:585:TYR:CD2	3:F:1302:HOH:O	2.46	0.66
1:B:791:GLU:OE1	3:B:1236:HOH:O	2.12	0.66
1:B:982:LEU:C	1:B:983:ILE:HD12	2.21	0.66
1:C:51:ASP:HA	1:C:66:LEU:HD12	1.76	0.66
1:B:766:ALA:HB3	1:B:793:SER:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:PHE:HD1	3:C:1298:HOH:O	1.77	0.66
1:A:468:LYS:HD2	1:A:473:ASP:HB3	1.76	0.66
1:B:51:ASP:HA	1:B:66:LEU:HD12	1.77	0.66
1:C:231:HIS:CE1	3:C:1274:HOH:O	2.47	0.66
1:D:364:ILE:O	3:D:1325:HOH:O	2.12	0.66
1:A:322:PRO:HA	1:A:678:LEU:HD22	1.77	0.66
1:E:976:LYS:HZ1	1:E:1017:ASP:HB2	1.59	0.66
1:B:929:MET:HE3	1:B:979:LEU:HD11	1.78	0.66
1:C:447:ALA:N	3:C:1263:HOH:O	2.29	0.66
1:B:61:LEU:HD13	1:B:74:ILE:HD11	1.78	0.66
1:C:468:LYS:HD2	1:C:473:ASP:HB3	1.78	0.66
1:E:446:GLU:OE1	1:E:468:LYS:HE2	1.96	0.66
1:A:589:ILE:HD13	1:A:641:LEU:HD22	1.79	0.65
1:C:233:SER:OG	3:C:1223:HOH:O	2.13	0.65
1:F:286:LEU:HD12	1:F:294:TYR:O	1.95	0.65
1:F:280:THR:HA	3:F:1265:HOH:O	1.96	0.65
1:F:82:ASN:H	1:F:82:ASN:HD22	1.44	0.65
1:B:225:ILE:HG13	1:B:226:VAL:HG23	1.77	0.65
1:C:225:ILE:HG13	1:C:226:VAL:HG23	1.79	0.65
1:C:913:ARG:HH21	1:C:1047:GLN:HE21	1.43	0.65
1:E:913:ARG:HH21	1:E:1047:GLN:HE21	1.45	0.65
1:A:82:ASN:HD22	1:A:82:ASN:H	1.44	0.65
1:C:196:THR:C	3:C:1274:HOH:O	2.38	0.65
1:C:921:SER:HB2	3:C:1252:HOH:O	1.96	0.65
1:F:766:ALA:HB3	1:F:793:SER:HA	1.78	0.65
1:F:929:MET:HE3	1:F:979:LEU:HD11	1.77	0.65
1:A:382:ARG:HA	3:A:1224:HOH:O	1.96	0.65
1:E:766:ALA:HB3	1:E:793:SER:HA	1.79	0.65
1:F:965:SER:CA	2:F:1214:DKT:O1	2.44	0.65
1:C:558:SER:C	3:C:1220:HOH:O	2.40	0.65
1:F:367:VAL:O	1:F:368:ARG:HD3	1.96	0.65
1:F:446:GLU:OE1	1:F:468:LYS:HE2	1.96	0.65
1:C:982:LEU:C	1:C:983:ILE:HD12	2.22	0.65
1:D:61:LEU:HB3	1:D:75:VAL:HG13	1.78	0.65
1:A:403:ASN:HD22	1:A:403:ASN:C	2.05	0.65
1:A:892:LEU:HD13	1:A:920:VAL:HG21	1.79	0.65
1:E:202:TRP:CH2	1:E:745:SER:HB3	2.32	0.65
1:E:403:ASN:HD22	1:E:403:ASN:C	2.03	0.65
1:A:766:ALA:HB3	1:A:793:SER:HA	1.77	0.64
1:B:190:ARG:HG3	1:B:216:GLU:OE2	1.96	0.64
1:B:1000:LEU:HD12	1:B:1004:THR:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:THR:HG22	1:D:303:ILE:CD1	2.26	0.64
1:F:351:SER:OG	1:F:353:THR:HG22	1.95	0.64
1:A:982:LEU:C	1:A:983:ILE:HD12	2.21	0.64
1:B:897:ARG:NE	3:B:1216:HOH:O	2.29	0.64
1:D:766:ALA:HB3	1:D:793:SER:HA	1.79	0.64
1:A:202:TRP:CH2	1:A:745:SER:HB3	2.33	0.64
1:A:913:ARG:HH21	1:A:1047:GLN:HE21	1.45	0.64
1:C:969:ILE:HG13	3:C:1276:HOH:O	1.97	0.64
1:F:430:THR:HG23	1:F:441:ILE:HD11	1.79	0.64
1:B:268:THR:HG22	1:B:303:ILE:CD1	2.28	0.64
1:C:589:ILE:HD13	1:C:641:LEU:HD22	1.79	0.64
1:F:225:ILE:HG13	1:F:226:VAL:HG23	1.79	0.64
1:A:268:THR:HG22	1:A:303:ILE:CD1	2.27	0.64
1:D:892:LEU:HB3	3:D:1321:HOH:O	1.96	0.64
1:F:713:ARG:NH1	3:F:1231:HOH:O	2.29	0.64
1:E:530:ASN:ND2	1:E:531:PHE:N	2.45	0.64
1:F:710:ILE:O	1:F:714:ILE:HG12	1.98	0.64
1:F:892:LEU:HD13	1:F:920:VAL:HG21	1.78	0.64
2:A:1214:DKT:C8	3:A:1308:HOH:O	2.45	0.64
1:E:710:ILE:O	1:E:714:ILE:HG12	1.97	0.64
1:F:51:ASP:HA	1:F:66:LEU:HD12	1.79	0.64
1:A:929:MET:HE3	1:A:979:LEU:HD11	1.79	0.64
1:E:268:THR:HG22	1:E:303:ILE:CD1	2.27	0.64
1:E:430:THR:HG23	1:E:441:ILE:HD11	1.80	0.64
1:A:190:ARG:HG3	1:A:216:GLU:OE2	1.98	0.64
1:B:155:PRO:O	1:B:856:ARG:HD2	1.98	0.64
1:B:710:ILE:O	1:B:714:ILE:HG12	1.98	0.64
1:C:568:LEU:HB3	1:C:571:MET:HE2	1.79	0.64
1:C:892:LEU:HD13	1:C:920:VAL:HG21	1.80	0.64
1:E:930:ASN:HD21	1:F:926:GLU:HG3	1.63	0.64
1:C:155:PRO:O	1:C:856:ARG:HD2	1.98	0.63
1:C:530:ASN:HD22	1:C:531:PHE:H	1.46	0.63
1:D:82:ASN:HD22	1:D:82:ASN:H	1.45	0.63
1:A:965:SER:CA	2:A:1214:DKT:O1	2.45	0.63
1:C:286:LEU:HD12	1:C:294:TYR:O	1.97	0.63
1:A:1000:LEU:HD12	1:A:1004:THR:HB	1.79	0.63
1:A:332:LEU:HD11	1:A:338:ALA:HB2	1.79	0.63
1:A:522:PRO:HG2	1:B:889:MET:SD	2.38	0.63
1:A:922:GLN:NE2	1:B:948:THR:H	1.96	0.63
1:C:430:THR:HG23	1:C:441:ILE:HD11	1.79	0.63
1:E:929:MET:HE3	1:E:979:LEU:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:467:LEU:C	3:F:1283:HOH:O	2.41	0.63
1:C:1045:ASP:HB3	1:C:1048:ILE:HG22	1.81	0.63
1:E:1000:LEU:HD12	1:E:1004:THR:HB	1.79	0.63
1:F:123:TYR:OH	1:F:823:ARG:HD3	1.99	0.63
1:F:739:GLN:NE2	3:F:1255:HOH:O	2.32	0.63
1:F:982:LEU:C	1:F:983:ILE:HD12	2.23	0.63
1:A:710:ILE:O	1:A:714:ILE:HG12	1.99	0.63
1:C:361:PRO:HG2	1:C:379:HIS:NE2	2.14	0.63
1:D:104:ASN:H	1:D:104:ASN:HD22	1.47	0.63
1:E:589:ILE:HB	1:E:596:LEU:HB2	1.81	0.63
1:F:430:THR:C	3:F:1276:HOH:O	2.42	0.63
1:F:467:LEU:O	3:F:1283:HOH:O	2.16	0.63
1:A:446:GLU:OE1	1:A:468:LYS:HE2	1.99	0.63
1:D:681:SER:HB3	1:D:684:GLU:HG2	1.81	0.63
1:D:1000:LEU:HD12	1:D:1004:THR:HB	1.80	0.63
1:F:65:ASP:HA	3:F:1222:HOH:O	1.98	0.63
1:C:1000:LEU:HD12	1:C:1004:THR:HB	1.80	0.62
1:A:51:ASP:HA	1:A:66:LEU:HD12	1.81	0.62
1:D:367:VAL:O	1:D:368:ARG:HD3	1.99	0.62
1:D:508:ASP:HB3	1:D:510:LYS:HE2	1.81	0.62
1:D:892:LEU:HD13	1:D:920:VAL:HG21	1.80	0.62
1:E:361:PRO:HG2	1:E:379:HIS:NE2	2.13	0.62
1:E:508:ASP:HB3	1:E:510:LYS:HE2	1.82	0.62
1:F:951:VAL:O	3:F:1281:HOH:O	2.16	0.62
1:C:939:ARG:HB2	3:C:1231:HOH:O	1.99	0.62
1:F:39:MET:N	3:F:1260:HOH:O	2.32	0.62
1:F:890:MET:HB3	3:F:1304:HOH:O	2.00	0.62
1:F:446:GLU:HG3	3:F:1283:HOH:O	1.99	0.62
1:A:940:ARG:HD2	3:A:1290:HOH:O	1.99	0.62
1:B:332:LEU:HD11	1:B:338:ALA:HB2	1.81	0.62
1:C:202:TRP:CH2	1:C:745:SER:HB3	2.35	0.62
1:C:373:THR:HG21	1:C:393:ARG:HD2	1.81	0.62
1:C:522:PRO:HG2	1:D:889:MET:SD	2.40	0.62
1:F:868:ARG:NH2	3:F:1315:HOH:O	2.33	0.62
1:B:589:ILE:HD13	1:B:641:LEU:HD22	1.81	0.62
1:C:61:LEU:HD13	1:C:74:ILE:HD11	1.81	0.62
1:F:361:PRO:HG2	1:F:379:HIS:NE2	2.15	0.62
1:F:399:LYS:HB2	3:F:1258:HOH:O	2.00	0.62
1:B:403:ASN:HD22	1:B:403:ASN:C	2.07	0.62
1:D:286:LEU:HD12	1:D:294:TYR:O	1.99	0.62
1:D:681:SER:CB	1:D:684:GLU:HG2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:891:GLY:HA3	3:E:1244:HOH:O	1.98	0.62
1:E:982:LEU:C	1:E:983:ILE:HD12	2.24	0.62
1:F:147:ILE:HG22	3:F:1293:HOH:O	1.99	0.62
1:F:589:ILE:HD13	1:F:641:LEU:HD22	1.81	0.62
1:B:49:HIS:CG	3:B:1225:HOH:O	2.52	0.62
1:B:430:THR:HG23	1:B:441:ILE:HD11	1.82	0.62
1:F:190:ARG:HG3	1:F:216:GLU:OE2	1.99	0.62
1:A:596:LEU:HD11	1:A:662:LEU:CD1	2.29	0.61
1:E:104:ASN:HD22	1:E:104:ASN:H	1.48	0.61
1:F:1000:LEU:HD12	1:F:1004:THR:HB	1.81	0.61
1:F:1008:GLN:NE2	3:F:1317:HOH:O	2.32	0.61
1:A:367:VAL:O	1:A:368:ARG:HD3	1.99	0.61
1:A:403:ASN:HD22	1:A:405:GLY:H	1.48	0.61
1:F:599:SER:CB	3:F:1302:HOH:O	2.48	0.61
1:A:593:SER:O	1:A:624:VAL:HG22	2.01	0.61
1:B:82:ASN:HD22	1:B:82:ASN:H	1.47	0.61
1:E:965:SER:C	2:E:1214:DKT:O1	2.43	0.61
1:F:944:SER:N	3:F:1254:HOH:O	2.22	0.61
1:A:286:LEU:HD12	1:A:294:TYR:O	1.99	0.61
1:B:892:LEU:HD13	1:B:920:VAL:HG21	1.82	0.61
1:C:367:VAL:O	1:C:368:ARG:HD3	2.01	0.61
1:D:104:ASN:H	1:D:104:ASN:ND2	1.99	0.61
1:E:82:ASN:H	1:E:82:ASN:HD22	1.48	0.61
1:E:330:SER:HB3	3:E:1260:HOH:O	1.98	0.61
1:F:61:LEU:HD13	1:F:74:ILE:HD11	1.81	0.61
1:A:530:ASN:ND2	1:A:531:PHE:N	2.49	0.61
1:E:286:LEU:HD12	1:E:294:TYR:O	2.01	0.61
1:F:681:SER:CB	1:F:684:GLU:HG2	2.31	0.61
1:F:681:SER:HB3	1:F:684:GLU:HG2	1.83	0.61
1:A:48:ILE:HB	1:A:286:LEU:HD22	1.83	0.61
1:A:225:ILE:HG13	1:A:226:VAL:HG23	1.83	0.61
1:B:556:PRO:HD3	1:D:354:TYR:CD1	2.35	0.61
1:E:74:ILE:HG13	1:E:75:VAL:HG12	1.81	0.61
1:B:367:VAL:O	1:B:368:ARG:HD3	2.01	0.61
1:E:892:LEU:HD13	1:E:920:VAL:HG21	1.83	0.61
1:F:373:THR:HG21	1:F:393:ARG:HD2	1.83	0.61
1:D:330:SER:HB3	3:D:1273:HOH:O	2.01	0.61
1:B:1048:ILE:O	1:B:1052:ILE:HG12	2.01	0.60
1:A:524:PRO:HD3	1:B:605:GLU:CG	2.30	0.60
1:D:361:PRO:HG2	1:D:379:HIS:NE2	2.17	0.60
1:D:589:ILE:HD13	1:D:641:LEU:HD22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ILE:HG13	1:A:75:VAL:HG12	1.83	0.60
1:A:361:PRO:HG2	1:A:379:HIS:NE2	2.16	0.60
1:B:202:TRP:CH2	1:B:745:SER:HB3	2.36	0.60
1:A:589:ILE:HB	1:A:596:LEU:HB2	1.82	0.60
1:A:605:GLU:CG	1:B:524:PRO:HD3	2.31	0.60
1:C:221:ALA:HB1	3:C:1327:HOH:O	2.00	0.60
1:C:710:ILE:O	1:C:714:ILE:HG12	2.00	0.60
1:D:206:ARG:N	1:D:1024:ASN:HD21	1.98	0.60
1:F:596:LEU:HD11	1:F:662:LEU:CD1	2.32	0.60
1:C:423:ASN:ND2	1:C:427:GLU:H	2.00	0.60
1:A:167:ASN:CB	3:A:1301:HOH:O	2.50	0.60
1:C:245:ILE:HD11	1:C:278:LEU:HG	1.84	0.60
1:C:403:ASN:HD22	1:C:405:GLY:H	1.47	0.60
1:C:964:GLY:O	3:C:1224:HOH:O	2.17	0.60
1:D:51:ASP:HA	1:D:66:LEU:HD12	1.83	0.60
1:D:171:ASN:CB	3:D:1215:HOH:O	2.08	0.60
1:F:202:TRP:CH2	1:F:745:SER:HB3	2.37	0.60
1:C:772:ASP:N	3:C:1234:HOH:O	2.35	0.60
1:C:959:THR:HG23	3:C:1247:HOH:O	2.01	0.60
1:D:589:ILE:HB	1:D:596:LEU:HB2	1.82	0.60
1:E:403:ASN:HD22	1:E:405:GLY:H	1.50	0.60
1:B:446:GLU:OE1	1:B:468:LYS:HE2	2.02	0.60
1:B:478:GLN:HB3	3:B:1270:HOH:O	2.01	0.60
1:C:189:ARG:O	3:C:1215:HOH:O	2.16	0.60
1:C:497:ASN:ND2	1:D:868:ARG:HH12	2.00	0.60
1:C:765:ILE:H	1:C:765:ILE:HD13	1.67	0.60
1:E:225:ILE:HG13	1:E:226:VAL:HG23	1.83	0.60
1:F:536:VAL:HB	3:F:1221:HOH:O	2.02	0.60
1:F:603:HIS:CD2	3:F:1235:HOH:O	2.54	0.60
1:D:596:LEU:HD11	1:D:662:LEU:CD1	2.32	0.60
1:E:367:VAL:O	1:E:368:ARG:HD3	2.00	0.60
1:A:965:SER:C	2:A:1214:DKT:O1	2.44	0.59
1:C:206:ARG:N	1:C:1024:ASN:HD21	1.97	0.59
1:C:1048:ILE:O	1:C:1052:ILE:HG12	2.01	0.59
1:D:123:TYR:OH	1:D:823:ARG:HD3	2.02	0.59
1:D:568:LEU:C	3:D:1256:HOH:O	2.45	0.59
1:F:666:GLU:HB3	3:F:1312:HOH:O	2.01	0.59
1:B:206:ARG:N	1:B:1024:ASN:HD21	1.95	0.59
1:F:206:ARG:N	1:F:1024:ASN:HD21	1.96	0.59
1:A:930:ASN:HD21	1:B:926:GLU:HG3	1.66	0.59
1:B:1045:ASP:HB3	1:B:1048:ILE:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:PRO:HD3	3:D:1321:HOH:O	2.01	0.59
1:C:589:ILE:HB	1:C:596:LEU:HB2	1.83	0.59
1:F:268:THR:HG22	1:F:303:ILE:CD1	2.32	0.59
1:A:446:GLU:HA	3:A:1296:HOH:O	2.01	0.59
1:B:286:LEU:HD12	1:B:294:TYR:O	2.02	0.59
1:F:517:TYR:C	3:F:1221:HOH:O	2.44	0.59
1:A:508:ASP:HB3	1:A:510:LYS:HE2	1.85	0.59
1:A:889:MET:SD	1:B:522:PRO:HG2	2.43	0.59
1:C:190:ARG:HG3	1:C:216:GLU:OE2	2.01	0.59
1:C:1027:VAL:CA	3:C:1217:HOH:O	2.49	0.59
1:D:104:ASN:ND2	3:D:1251:HOH:O	2.33	0.59
1:D:430:THR:HG23	1:D:441:ILE:HD11	1.83	0.59
1:E:51:ASP:HA	1:E:66:LEU:HD12	1.84	0.59
1:E:104:ASN:H	1:E:104:ASN:ND2	2.00	0.59
1:E:681:SER:HB3	1:E:684:GLU:HG2	1.84	0.59
1:A:155:PRO:O	1:A:856:ARG:HD2	2.01	0.59
1:A:430:THR:HG23	1:A:441:ILE:HD11	1.84	0.59
1:A:681:SER:HB3	1:A:684:GLU:HG2	1.85	0.59
1:A:744:THR:HG22	1:A:745:SER:N	2.17	0.59
1:C:618:VAL:HG23	1:C:633:LYS:O	2.03	0.59
1:A:1045:ASP:HB3	1:A:1048:ILE:HG22	1.85	0.59
1:B:508:ASP:HB3	1:B:510:LYS:HE2	1.84	0.59
1:B:530:ASN:HD22	1:B:531:PHE:H	1.51	0.59
1:C:771:LEU:HA	3:C:1234:HOH:O	2.01	0.59
1:D:202:TRP:CH2	1:D:745:SER:HB3	2.38	0.59
1:D:492:ALA:C	3:D:1221:HOH:O	2.44	0.59
1:E:184:LEU:HD21	3:E:1291:HOH:O	2.02	0.59
1:E:596:LEU:HD11	1:E:662:LEU:CD1	2.32	0.59
1:E:746:HIS:NE2	1:E:965:SER:OG	2.33	0.59
1:F:423:ASN:ND2	1:F:427:GLU:H	2.00	0.59
1:B:596:LEU:HD11	1:B:662:LEU:CD1	2.33	0.59
1:C:423:ASN:HD21	1:C:427:GLU:H	1.51	0.59
1:D:74:ILE:HG13	1:D:75:VAL:HG12	1.84	0.59
1:B:74:ILE:HG13	1:B:75:VAL:HG12	1.84	0.59
1:E:373:THR:HG21	1:E:393:ARG:HD2	1.84	0.59
1:F:722:VAL:N	1:F:723:PRO:HD2	2.18	0.59
1:A:430:THR:C	3:A:1249:HOH:O	2.45	0.58
1:D:640:ARG:O	3:D:1218:HOH:O	2.15	0.58
1:E:965:SER:CA	2:E:1214:DKT:O1	2.45	0.58
1:F:245:ILE:HD11	1:F:278:LEU:HG	1.85	0.58
1:F:593:SER:O	1:F:624:VAL:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:765:ILE:H	1:F:765:ILE:HD13	1.68	0.58
1:B:403:ASN:HD22	1:B:405:GLY:H	1.51	0.58
1:C:74:ILE:HG13	1:C:75:VAL:HG12	1.84	0.58
1:C:530:ASN:ND2	1:C:531:PHE:N	2.51	0.58
1:D:999:ARG:HG2	1:D:1005:VAL:HG22	1.85	0.58
1:E:681:SER:CB	1:E:684:GLU:HG2	2.33	0.58
1:F:1045:ASP:HB3	1:F:1048:ILE:HG22	1.84	0.58
1:A:337:ILE:HD12	1:A:649:MET:HE2	1.85	0.58
1:B:593:SER:O	1:B:624:VAL:HG22	2.03	0.58
1:C:268:THR:HG22	1:C:303:ILE:CD1	2.32	0.58
1:C:868:ARG:HH12	1:D:497:ASN:ND2	2.01	0.58
1:D:530:ASN:ND2	1:D:531:PHE:N	2.48	0.58
1:E:589:ILE:HD13	1:E:641:LEU:HD22	1.85	0.58
1:E:899:PHE:HE2	1:E:949:ASN:HD22	1.51	0.58
1:F:403:ASN:HD22	1:F:405:GLY:H	1.49	0.58
1:F:618:VAL:HG23	1:F:633:LYS:O	2.04	0.58
1:A:256:SER:OG	1:A:267:HIS:HE1	1.87	0.58
1:C:197:PHE:N	3:C:1274:HOH:O	2.36	0.58
1:D:423:ASN:ND2	1:D:427:GLU:H	2.02	0.58
1:E:245:ILE:HD11	1:E:278:LEU:HG	1.86	0.58
1:E:660:PHE:HB3	1:E:668:GLU:HB3	1.85	0.58
1:F:917:GLY:HA3	2:F:1214:DKT:O	2.03	0.58
1:F:965:SER:C	2:F:1214:DKT:O1	2.46	0.58
1:B:1002:ASP:HB2	3:B:1319:HOH:O	2.04	0.58
1:C:203:LYS:HG2	3:C:1337:HOH:O	2.02	0.58
1:B:589:ILE:HB	1:B:596:LEU:HB2	1.84	0.58
1:C:196:THR:HA	3:C:1274:HOH:O	2.04	0.58
1:F:74:ILE:HG13	1:F:75:VAL:HG12	1.84	0.58
1:D:203:LYS:HD3	1:D:274:TYR:CZ	2.38	0.58
1:E:423:ASN:ND2	1:E:427:GLU:H	2.02	0.58
1:E:917:GLY:HA3	2:E:1214:DKT:O	2.04	0.58
1:E:999:ARG:HG2	1:E:1005:VAL:HG22	1.85	0.58
1:F:1039:ASP:N	3:F:1267:HOH:O	2.31	0.58
1:B:284:ARG:CZ	3:B:1320:HOH:O	2.52	0.58
1:C:508:ASP:HB3	1:C:510:LYS:HE2	1.86	0.58
1:C:681:SER:CB	1:C:684:GLU:HG2	2.34	0.58
1:F:61:LEU:CB	1:F:75:VAL:HG13	2.34	0.58
1:F:337:ILE:HD12	1:F:649:MET:HE2	1.85	0.58
1:F:530:ASN:HD22	1:F:531:PHE:H	1.50	0.58
1:F:660:PHE:HB3	1:F:668:GLU:HB3	1.85	0.58
1:F:988:TRP:C	3:F:1256:HOH:O	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:917:GLY:HA3	2:C:1214:DKT:O	2.04	0.57
1:F:710:ILE:HD13	1:F:713:ARG:HH22	1.69	0.57
1:C:337:ILE:HD12	1:C:649:MET:HE2	1.84	0.57
1:D:203:LYS:HD3	1:D:274:TYR:CE1	2.40	0.57
1:A:373:THR:HG21	1:A:393:ARG:HD2	1.86	0.57
1:B:361:PRO:HG2	1:B:379:HIS:NE2	2.19	0.57
1:B:618:VAL:HG23	1:B:633:LYS:O	2.04	0.57
1:D:1048:ILE:O	1:D:1052:ILE:HG12	2.04	0.57
1:F:155:PRO:O	1:F:856:ARG:HD2	2.03	0.57
1:B:373:THR:HG21	1:B:393:ARG:HD2	1.85	0.57
1:B:423:ASN:ND2	1:B:427:GLU:H	2.03	0.57
1:B:917:GLY:HA3	2:B:1214:DKT:O	2.04	0.57
1:D:944:SER:N	3:D:1269:HOH:O	2.37	0.57
1:E:48:ILE:HB	1:E:286:LEU:HD22	1.86	0.57
1:E:123:TYR:OH	1:E:823:ARG:HD3	2.03	0.57
1:A:423:ASN:ND2	1:A:427:GLU:H	2.02	0.57
1:A:1048:ILE:O	1:A:1052:ILE:HG12	2.04	0.57
1:D:373:THR:HG21	1:D:393:ARG:HD2	1.84	0.57
1:C:596:LEU:HD11	1:C:662:LEU:CD1	2.33	0.57
1:C:346:PHE:HB2	3:C:1298:HOH:O	2.04	0.57
1:C:578:ILE:HD11	1:C:580:VAL:CG2	2.35	0.57
1:C:922:GLN:NE2	1:D:948:THR:H	2.00	0.57
1:D:225:ILE:HG13	1:D:226:VAL:HG23	1.87	0.57
1:D:710:ILE:O	1:D:714:ILE:HG12	2.04	0.57
1:E:578:ILE:HD11	1:E:580:VAL:CG2	2.35	0.57
1:A:40:PRO:HG2	1:A:724:LEU:CD2	2.34	0.57
1:A:61:LEU:CB	1:A:75:VAL:HG13	2.34	0.57
1:F:589:ILE:HB	1:F:596:LEU:HB2	1.85	0.57
1:B:48:ILE:HB	1:B:286:LEU:HD22	1.87	0.57
1:B:104:ASN:ND2	1:B:104:ASN:H	2.03	0.57
1:B:994:ILE:HD12	1:B:994:ILE:O	2.05	0.57
1:C:104:ASN:H	1:C:104:ASN:ND2	2.03	0.57
1:F:508:ASP:HB3	1:F:510:LYS:HE2	1.87	0.57
1:F:939:ARG:CZ	3:F:1216:HOH:O	2.50	0.57
1:A:556:PRO:HD3	1:E:354:TYR:CD1	2.39	0.57
1:B:681:SER:CB	1:B:684:GLU:HG2	2.35	0.57
1:D:593:SER:O	1:D:624:VAL:HG22	2.05	0.57
1:F:203:LYS:HD3	1:F:274:TYR:CE1	2.40	0.57
1:A:722:VAL:N	1:A:723:PRO:HD2	2.20	0.56
1:C:85:ARG:NH2	3:C:1245:HOH:O	2.38	0.56
1:C:660:PHE:HB3	1:C:668:GLU:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:917:GLY:HA3	2:D:1214:DKT:O	2.05	0.56
1:E:155:PRO:O	1:E:856:ARG:HD2	2.04	0.56
1:E:206:ARG:N	1:E:1024:ASN:HD21	2.02	0.56
1:A:164:ARG:HG3	3:A:1264:HOH:O	2.05	0.56
1:D:660:PHE:HB3	1:D:668:GLU:HB3	1.87	0.56
1:A:471:GLU:HG2	3:B:1256:HOH:O	2.04	0.56
1:A:618:VAL:HG23	1:A:633:LYS:O	2.05	0.56
1:B:49:HIS:CE1	3:B:1225:HOH:O	2.59	0.56
1:B:307:GLU:HA	3:B:1259:HOH:O	2.04	0.56
1:B:489:LYS:HG3	1:B:491:PHE:CE1	2.40	0.56
1:C:367:VAL:N	3:C:1251:HOH:O	2.38	0.56
1:C:442:GLU:C	3:C:1267:HOH:O	2.48	0.56
1:C:970:PHE:CA	3:C:1252:HOH:O	2.50	0.56
1:D:403:ASN:HD22	1:D:405:GLY:H	1.50	0.56
1:E:61:LEU:HD13	1:E:74:ILE:CD1	2.36	0.56
1:E:423:ASN:HD21	1:E:427:GLU:H	1.52	0.56
1:F:242:ILE:O	1:F:256:SER:HA	2.05	0.56
1:B:314:PRO:HA	1:E:118:ILE:HG22	1.86	0.56
1:C:786:TYR:HB3	3:D:1252:HOH:O	2.06	0.56
1:D:722:VAL:N	1:D:723:PRO:HD2	2.20	0.56
1:F:423:ASN:HD21	1:F:427:GLU:H	1.51	0.56
1:B:744:THR:HG22	1:B:745:SER:N	2.21	0.56
1:C:690:TYR:HD1	3:C:1306:HOH:O	1.87	0.56
1:F:1048:ILE:O	1:F:1052:ILE:HG12	2.06	0.56
1:A:578:ILE:O	1:A:578:ILE:HG13	2.04	0.56
1:A:681:SER:CB	1:A:684:GLU:HG2	2.35	0.56
1:A:899:PHE:HE2	1:A:949:ASN:HD22	1.53	0.56
1:B:256:SER:OG	1:B:267:HIS:HE1	1.88	0.56
1:B:899:PHE:HE2	1:B:949:ASN:HD22	1.54	0.56
1:C:365:ARG:HG2	1:C:365:ARG:HH21	1.71	0.56
3:C:1233:HOH:O	1:D:976:LYS:HE2	2.05	0.56
1:D:431:VAL:C	3:D:1262:HOH:O	2.48	0.56
1:F:203:LYS:HD3	1:F:274:TYR:CZ	2.41	0.56
1:A:917:GLY:HA3	2:A:1214:DKT:O	2.05	0.56
1:B:710:ILE:HD13	1:B:713:ARG:HH22	1.71	0.56
1:B:999:ARG:HG2	1:B:1005:VAL:HG22	1.88	0.56
1:C:899:PHE:HE2	1:C:949:ASN:HD22	1.54	0.56
1:F:530:ASN:ND2	1:F:531:PHE:N	2.53	0.56
1:A:61:LEU:HD13	1:A:74:ILE:CD1	2.36	0.56
1:C:61:LEU:CB	1:C:75:VAL:HG13	2.36	0.56
1:C:429:MET:HG3	3:C:1227:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:959:THR:C	3:C:1247:HOH:O	2.49	0.56
1:F:744:THR:HG22	1:F:745:SER:N	2.20	0.56
1:C:242:ILE:O	1:C:256:SER:HA	2.05	0.56
1:C:681:SER:HB3	1:C:684:GLU:HG2	1.88	0.56
1:C:722:VAL:N	1:C:723:PRO:HD2	2.21	0.56
1:D:423:ASN:HD21	1:D:427:GLU:H	1.54	0.56
1:D:703:ASN:C	1:D:703:ASN:HD22	2.12	0.56
1:F:999:ARG:HG2	1:F:1005:VAL:HG22	1.88	0.56
1:A:258:ASP:C	1:A:260:ASP:H	2.14	0.56
1:B:104:ASN:H	1:B:104:ASN:HD22	1.54	0.56
1:B:203:LYS:HD3	1:B:274:TYR:CZ	2.41	0.56
1:E:242:ILE:O	1:E:256:SER:HA	2.06	0.56
1:E:645:ARG:HH21	1:E:645:ARG:HG3	1.70	0.56
1:F:346:PHE:HB3	3:F:1299:HOH:O	2.06	0.56
1:B:123:TYR:OH	1:B:823:ARG:HD3	2.06	0.55
1:B:722:VAL:N	1:B:723:PRO:HD2	2.22	0.55
1:C:710:ILE:HD13	1:C:713:ARG:HH22	1.70	0.55
1:E:578:ILE:HG13	1:E:578:ILE:O	2.06	0.55
1:A:417:LYS:HD2	3:A:1222:HOH:O	2.06	0.55
1:B:765:ILE:HD13	1:B:765:ILE:H	1.70	0.55
1:A:203:LYS:HD3	1:A:274:TYR:CZ	2.42	0.55
1:D:218:ASN:HA	3:D:1340:HOH:O	2.07	0.55
1:D:765:ILE:HD11	1:D:769:PHE:HZ	1.72	0.55
1:E:965:SER:HG	2:E:1214:DKT:C7	2.11	0.55
1:D:61:LEU:HD13	1:D:74:ILE:CD1	2.36	0.55
1:F:104:ASN:ND2	1:F:104:ASN:H	2.03	0.55
1:B:681:SER:HB3	1:B:684:GLU:HG2	1.86	0.55
1:C:104:ASN:H	1:C:104:ASN:HD22	1.53	0.55
1:D:774:ASP:HA	1:D:817:ALA:HB2	1.89	0.55
1:E:203:LYS:HD3	1:E:274:TYR:CE1	2.41	0.55
1:E:442:GLU:HG3	3:E:1242:HOH:O	2.06	0.55
1:D:943:LEU:HB3	3:D:1269:HOH:O	2.07	0.55
1:E:703:ASN:HD22	1:E:703:ASN:C	2.14	0.55
1:F:360:GLU:OE2	1:F:361:PRO:HD2	2.07	0.55
1:F:703:ASN:C	1:F:703:ASN:HD22	2.14	0.55
1:A:164:ARG:CD	3:A:1264:HOH:O	2.54	0.55
1:B:61:LEU:CB	1:B:75:VAL:HG13	2.34	0.55
1:E:765:ILE:HD13	3:E:1227:HOH:O	2.05	0.55
1:A:123:TYR:OH	1:A:823:ARG:HD3	2.07	0.55
1:B:40:PRO:HG2	1:B:724:LEU:CD2	2.35	0.55
1:C:440:VAL:N	3:C:1312:HOH:O	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:PHE:HB3	1:C:463:TYR:HB3	1.89	0.55
1:D:155:PRO:O	1:D:856:ARG:HD2	2.07	0.55
1:A:104:ASN:ND2	1:A:104:ASN:H	2.05	0.55
1:C:203:LYS:HD3	1:C:274:TYR:CZ	2.41	0.55
1:C:578:ILE:HG13	1:C:578:ILE:O	2.05	0.55
1:C:939:ARG:CA	3:C:1231:HOH:O	2.55	0.55
1:F:519:SER:N	3:F:1221:HOH:O	2.39	0.55
1:B:245:ILE:HD11	1:B:278:LEU:HG	1.89	0.55
1:B:258:ASP:C	1:B:260:ASP:H	2.15	0.55
1:C:999:ARG:HG2	1:C:1005:VAL:HG22	1.88	0.55
1:E:203:LYS:HD3	1:E:274:TYR:CZ	2.42	0.55
1:F:258:ASP:C	1:F:260:ASP:H	2.15	0.55
1:F:452:PHE:HB3	1:F:463:TYR:HB3	1.88	0.55
1:F:104:ASN:H	1:F:104:ASN:HD22	1.55	0.54
1:F:201:HIS:CE1	3:F:1282:HOH:O	2.60	0.54
1:A:245:ILE:HD11	1:A:278:LEU:HG	1.88	0.54
1:B:452:PHE:HB3	1:B:463:TYR:HB3	1.89	0.54
1:C:558:SER:CB	3:C:1220:HOH:O	2.55	0.54
1:D:82:ASN:HD21	1:D:96:ARG:HH21	1.55	0.54
1:B:337:ILE:HD12	1:B:649:MET:HE2	1.86	0.54
1:C:197:PHE:O	3:C:1274:HOH:O	2.17	0.54
1:C:948:THR:H	1:D:922:GLN:NE2	2.01	0.54
1:D:572:TYR:O	3:D:1252:HOH:O	2.18	0.54
1:B:61:LEU:HD13	1:B:74:ILE:CD1	2.37	0.54
1:C:238:VAL:HG11	1:C:298:PRO:HG2	1.89	0.54
1:E:337:ILE:HD12	1:E:649:MET:HE2	1.88	0.54
1:E:707:ALA:CB	3:F:1216:HOH:O	2.54	0.54
1:A:660:PHE:HB3	1:A:668:GLU:HB3	1.88	0.54
1:A:765:ILE:H	1:A:765:ILE:HD13	1.71	0.54
1:C:203:LYS:HD3	1:C:274:TYR:CE1	2.42	0.54
1:C:498:SER:OG	1:C:518:ARG:HG2	2.08	0.54
1:E:722:VAL:N	1:E:723:PRO:HD2	2.23	0.54
1:C:162:LEU:HD21	1:C:180:ALA:HB3	1.89	0.54
1:C:480:ILE:HB	1:C:493:ALA:HB3	1.89	0.54
1:D:765:ILE:HD11	1:D:769:PHE:CZ	2.42	0.54
1:E:40:PRO:HG2	1:E:724:LEU:CD2	2.37	0.54
1:B:203:LYS:HD3	1:B:274:TYR:CE1	2.43	0.54
1:C:360:GLU:OE2	1:C:361:PRO:HD2	2.07	0.54
1:A:999:ARG:HG2	1:A:1005:VAL:HG22	1.90	0.54
1:B:660:PHE:HB3	1:B:668:GLU:HB3	1.89	0.54
1:D:105:THR:OG1	3:D:1297:HOH:O	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:ARG:NH2	1:D:166:GLU:OE1	2.39	0.54
1:D:218:ASN:CB	3:D:1258:HOH:O	2.49	0.54
1:E:618:VAL:HG23	1:E:633:LYS:O	2.08	0.54
1:E:765:ILE:HD11	1:E:769:PHE:HZ	1.73	0.54
1:C:180:ALA:C	3:C:1311:HOH:O	2.51	0.54
1:D:618:VAL:HG23	1:D:633:LYS:O	2.08	0.54
1:E:164:ARG:NH2	1:E:166:GLU:OE1	2.41	0.54
1:F:48:ILE:HB	1:F:286:LEU:HD22	1.90	0.54
1:F:645:ARG:HH21	1:F:645:ARG:HG3	1.73	0.54
1:A:82:ASN:HD21	1:A:96:ARG:HG2	1.73	0.53
1:A:242:ILE:O	1:A:256:SER:HA	2.07	0.53
1:C:593:SER:O	1:C:624:VAL:HG22	2.07	0.53
1:C:994:ILE:HD12	1:C:994:ILE:O	2.08	0.53
1:D:1045:ASP:HB3	1:D:1048:ILE:HG22	1.89	0.53
1:E:593:SER:O	1:E:624:VAL:HG22	2.09	0.53
1:C:258:ASP:C	1:C:260:ASP:H	2.16	0.53
1:C:473:ASP:HA	1:D:904:SER:OG	2.07	0.53
2:A:1214:DKT:CE6	3:A:1276:HOH:O	2.29	0.53
1:C:744:THR:HG22	1:C:745:SER:N	2.23	0.53
1:D:284:ARG:HD3	3:D:1227:HOH:O	2.07	0.53
1:E:765:ILE:HD13	1:E:765:ILE:H	1.73	0.53
1:E:868:ARG:HH12	1:F:497:ASN:ND2	2.06	0.53
1:F:365:ARG:HG2	1:F:365:ARG:HH21	1.72	0.53
1:A:774:ASP:HA	1:A:817:ALA:HB2	1.90	0.53
1:C:703:ASN:HD22	1:C:703:ASN:C	2.15	0.53
1:D:61:LEU:CB	1:D:75:VAL:HG13	2.38	0.53
1:E:499:HIS:CD2	3:E:1221:HOH:O	2.58	0.53
1:A:145:ASN:HB2	3:A:1264:HOH:O	2.07	0.53
1:B:1031:VAL:HG12	1:B:1033:ILE:CD1	2.39	0.53
1:C:228:MET:HE1	1:C:244:PHE:CZ	2.43	0.53
1:D:48:ILE:HB	1:D:286:LEU:HD22	1.90	0.53
1:D:645:ARG:HH21	1:D:645:ARG:HG3	1.73	0.53
1:D:744:THR:HG22	1:D:745:SER:N	2.23	0.53
1:F:238:VAL:HG11	1:F:298:PRO:HG2	1.89	0.53
1:B:87:PHE:CB	1:B:88:PRO:HD2	2.38	0.53
1:C:85:ARG:CZ	3:C:1245:HOH:O	2.56	0.53
1:E:1045:ASP:HB3	1:E:1048:ILE:HG22	1.91	0.53
1:C:837:LEU:HB2	1:C:845:ARG:HB2	1.90	0.53
1:D:765:ILE:HD13	1:D:765:ILE:H	1.73	0.53
1:D:986:ARG:HA	1:D:1027:VAL:O	2.09	0.53
1:E:228:MET:HE1	1:E:244:PHE:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1048:ILE:O	1:E:1052:ILE:HG12	2.09	0.53
1:F:138:ALA:CB	3:F:1293:HOH:O	2.57	0.53
1:B:423:ASN:HD21	1:B:427:GLU:H	1.54	0.53
1:B:913:ARG:HH21	1:B:1047:GLN:HE21	1.56	0.53
1:C:61:LEU:HD13	1:C:74:ILE:CD1	2.39	0.53
1:D:258:ASP:C	1:D:260:ASP:H	2.15	0.53
1:E:61:LEU:CB	1:E:75:VAL:HG13	2.38	0.53
1:E:645:ARG:HG3	1:E:645:ARG:NH2	2.23	0.53
1:A:104:ASN:H	1:A:104:ASN:HD22	1.57	0.53
1:A:524:PRO:HD3	1:B:605:GLU:HG3	1.89	0.53
1:A:746:HIS:CE1	1:A:965:SER:OG	2.62	0.53
1:E:82:ASN:HD21	1:E:96:ARG:HH21	1.57	0.53
1:E:360:GLU:OE2	1:E:361:PRO:HD2	2.08	0.53
1:E:1031:VAL:HG12	1:E:1033:ILE:CD1	2.39	0.53
1:A:228:MET:HE1	1:A:244:PHE:CZ	2.43	0.53
1:A:605:GLU:HG3	1:B:524:PRO:HD3	1.90	0.53
1:E:994:ILE:HD12	1:E:994:ILE:O	2.08	0.53
1:A:823:ARG:HD2	1:D:317:ARG:HD3	1.92	0.52
1:B:242:ILE:O	1:B:256:SER:HA	2.08	0.52
1:D:337:ILE:HD12	1:D:649:MET:HE2	1.87	0.52
1:D:572:TYR:HB3	3:D:1221:HOH:O	2.08	0.52
1:E:222:PHE:H	1:E:1038:HIS:CD2	2.28	0.52
1:A:279:ASN:ND2	3:A:1273:HOH:O	2.42	0.52
1:B:365:ARG:HH21	1:B:365:ARG:HG2	1.75	0.52
1:C:164:ARG:NH2	1:C:166:GLU:OE1	2.42	0.52
1:C:498:SER:HB2	3:C:1320:HOH:O	2.09	0.52
1:D:627:ARG:C	3:D:1264:HOH:O	2.52	0.52
1:F:837:LEU:HB2	1:F:845:ARG:HB2	1.92	0.52
1:C:959:THR:O	1:C:984:GLY:HA3	2.09	0.52
1:D:245:ILE:HD11	1:D:278:LEU:HG	1.91	0.52
1:A:203:LYS:HD3	1:A:274:TYR:CE1	2.44	0.52
1:A:452:PHE:HB3	1:A:463:TYR:HB3	1.91	0.52
1:A:489:LYS:HG3	1:A:491:PHE:CE1	2.44	0.52
1:B:530:ASN:ND2	1:B:531:PHE:N	2.56	0.52
1:E:765:ILE:HD11	1:E:769:PHE:CZ	2.44	0.52
1:D:336:LEU:O	1:D:337:ILE:HD13	2.10	0.52
1:E:591:LEU:HD11	1:E:662:LEU:HD21	1.91	0.52
1:E:703:ASN:OD1	1:E:706:VAL:HG23	2.09	0.52
1:F:157:SER:HB2	3:F:1314:HOH:O	2.08	0.52
1:F:899:PHE:HE2	1:F:949:ASN:HD22	1.58	0.52
1:A:926:GLU:HG3	1:B:930:ASN:HD21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LEU:HD23	1:B:287:PHE:HB3	1.91	0.52
1:C:124:PHE:HB3	1:C:152:ALA:CB	2.39	0.52
1:E:744:THR:HG22	1:E:745:SER:N	2.25	0.52
1:F:599:SER:HA	3:F:1302:HOH:O	2.08	0.52
1:F:642:SER:HB3	1:F:647:THR:HB	1.92	0.52
1:A:314:PRO:HA	1:D:118:ILE:HG22	1.91	0.52
1:B:228:MET:HE1	1:B:244:PHE:CZ	2.44	0.52
1:C:774:ASP:HA	1:C:817:ALA:HB2	1.92	0.52
1:E:926:GLU:HG3	1:F:930:ASN:HD21	1.74	0.52
1:F:256:SER:OG	1:F:267:HIS:HE1	1.93	0.52
1:F:541:VAL:HG22	1:F:542:ILE:N	2.25	0.52
1:A:471:GLU:CG	3:B:1256:HOH:O	2.57	0.52
1:C:278:LEU:HD23	1:C:287:PHE:HB3	1.92	0.52
1:D:452:PHE:HB3	1:D:463:TYR:HB3	1.92	0.52
1:D:703:ASN:OD1	1:D:706:VAL:HG23	2.10	0.52
1:E:452:PHE:HB3	1:E:463:TYR:HB3	1.91	0.52
1:F:645:ARG:HG3	1:F:645:ARG:NH2	2.25	0.52
1:F:728:ARG:HG3	1:F:754:PHE:CE1	2.45	0.52
1:A:604:GLY:HA3	1:B:521:ASP:OD1	2.10	0.52
1:A:703:ASN:C	1:A:703:ASN:HD22	2.18	0.52
1:E:887:MET:O	1:E:920:VAL:HG22	2.09	0.52
1:F:278:LEU:HD23	1:F:287:PHE:HB3	1.91	0.52
1:A:360:GLU:OE2	1:A:361:PRO:HD2	2.10	0.52
1:A:959:THR:O	1:A:984:GLY:HA3	2.10	0.52
1:C:541:VAL:HG22	1:C:542:ILE:N	2.25	0.52
1:A:190:ARG:C	3:A:1266:HOH:O	2.53	0.51
1:A:423:ASN:HD21	1:A:427:GLU:H	1.55	0.51
1:A:524:PRO:HD3	1:B:605:GLU:HG2	1.92	0.51
1:B:774:ASP:HA	1:B:817:ALA:HB2	1.92	0.51
1:B:959:THR:O	1:B:984:GLY:HA3	2.10	0.51
1:C:916:GLY:C	3:C:1224:HOH:O	2.52	0.51
1:D:242:ILE:O	1:D:256:SER:HA	2.10	0.51
1:D:899:PHE:HE2	1:D:949:ASN:HD22	1.58	0.51
1:E:774:ASP:HA	1:E:817:ALA:HB2	1.90	0.51
1:A:936:ASP:HB2	3:A:1281:HOH:O	2.10	0.51
1:C:926:GLU:HG3	1:D:930:ASN:HD21	1.76	0.51
1:C:955:ILE:HB	3:C:1316:HOH:O	2.10	0.51
1:E:238:VAL:HG11	1:E:298:PRO:HG2	1.92	0.51
1:E:353:THR:HG23	1:E:354:TYR:CD1	2.45	0.51
1:E:525:ASP:HB2	1:F:532:SER:HB2	1.92	0.51
1:E:802:PRO:O	1:E:805:TYR:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:PRO:HD2	1:D:827:GLU:O	2.10	0.51
1:A:764:ARG:NH2	3:A:1289:HOH:O	2.44	0.51
1:D:645:ARG:HB2	3:D:1342:HOH:O	2.10	0.51
1:E:986:ARG:HA	1:E:1027:VAL:O	2.10	0.51
1:F:480:ILE:HB	1:F:493:ALA:HB3	1.92	0.51
1:F:550:ASN:C	1:F:550:ASN:OD1	2.53	0.51
1:A:278:LEU:HD23	1:A:287:PHE:HB3	1.91	0.51
1:A:867:ASN:HD22	1:A:867:ASN:N	2.08	0.51
1:C:645:ARG:HG3	1:C:645:ARG:HH21	1.76	0.51
1:A:238:VAL:HG11	1:A:298:PRO:HG2	1.92	0.51
1:A:550:ASN:C	1:A:550:ASN:OD1	2.54	0.51
1:A:1031:VAL:HG12	1:A:1033:ILE:CD1	2.41	0.51
1:B:578:ILE:HG13	1:B:578:ILE:O	2.09	0.51
1:D:228:MET:HE1	1:D:244:PHE:CZ	2.45	0.51
1:E:124:PHE:HB3	1:E:152:ALA:CB	2.40	0.51
1:E:317:ARG:NH1	3:E:1226:HOH:O	2.42	0.51
1:E:336:LEU:O	1:E:337:ILE:HD13	2.10	0.51
1:A:994:ILE:O	1:A:994:ILE:HD12	2.10	0.51
1:C:904:SER:OG	1:D:473:ASP:HA	2.10	0.51
1:D:530:ASN:HD22	1:D:531:PHE:N	2.09	0.51
1:D:959:THR:O	1:D:984:GLY:HA3	2.11	0.51
1:E:959:THR:O	1:E:984:GLY:HA3	2.11	0.51
1:A:143:ASP:CG	3:A:1291:HOH:O	2.54	0.51
1:C:373:THR:HG22	1:E:558:SER:HB2	1.93	0.51
1:E:256:SER:OG	1:E:267:HIS:HE1	1.93	0.51
1:F:764:ARG:HG3	3:F:1247:HOH:O	2.10	0.51
1:B:683:HIS:HB2	3:B:1295:HOH:O	2.10	0.51
1:D:578:ILE:HD11	1:D:580:VAL:CG2	2.38	0.51
1:E:258:ASP:C	1:E:260:ASP:H	2.18	0.51
1:E:546:PRO:HG2	1:E:567:ASP:HB3	1.93	0.51
1:F:61:LEU:HD13	1:F:74:ILE:CD1	2.41	0.51
1:B:82:ASN:HD21	1:B:96:ARG:HH21	1.59	0.51
1:D:867:ASN:N	1:D:867:ASN:HD22	2.09	0.51
1:B:802:PRO:O	1:B:805:TYR:HB2	2.11	0.50
1:C:444:SER:OG	1:C:466:PRO:HG2	2.11	0.50
1:C:802:PRO:O	1:C:805:TYR:HB2	2.10	0.50
1:D:278:LEU:HD23	1:D:287:PHE:HB3	1.92	0.50
1:E:131:ARG:HH21	1:E:131:ARG:HG2	1.75	0.50
1:F:48:ILE:HG21	3:F:1265:HOH:O	2.11	0.50
1:C:1028:ASP:N	3:C:1217:HOH:O	2.43	0.50
1:D:222:PHE:H	1:D:1038:HIS:CD2	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:558:SER:HB2	1:F:373:THR:HG22	1.92	0.50
1:F:124:PHE:HB3	1:F:152:ALA:CB	2.41	0.50
1:F:228:MET:HE1	1:F:244:PHE:CZ	2.46	0.50
1:B:317:ARG:CD	1:E:823:ARG:HD2	2.37	0.50
1:C:642:SER:HB3	1:C:647:THR:HB	1.94	0.50
1:E:225:ILE:O	1:E:261:GLY:HA3	2.11	0.50
1:E:362:LEU:HD13	1:E:688:GLN:HG3	1.93	0.50
1:F:222:PHE:H	1:F:1038:HIS:CD2	2.29	0.50
1:B:785:ASP:N	3:B:1236:HOH:O	2.43	0.50
1:D:225:ILE:O	1:D:261:GLY:HA3	2.11	0.50
1:D:353:THR:HG23	1:D:354:TYR:CD1	2.46	0.50
1:F:286:LEU:N	3:F:1265:HOH:O	2.43	0.50
1:F:543:PRO:HB3	3:F:1318:HOH:O	2.10	0.50
1:B:164:ARG:NH2	1:B:166:GLU:OE1	2.45	0.50
1:B:360:GLU:OE2	1:B:361:PRO:HD2	2.12	0.50
1:D:645:ARG:HG3	1:D:645:ARG:NH2	2.26	0.50
1:E:642:SER:HB3	1:E:647:THR:HB	1.93	0.50
1:F:791:GLU:CD	1:F:861:ARG:HE	2.19	0.50
1:F:994:ILE:HD12	1:F:994:ILE:O	2.12	0.50
1:B:541:VAL:HG22	1:B:542:ILE:N	2.27	0.50
1:C:189:ARG:C	3:C:1215:HOH:O	2.53	0.50
1:D:124:PHE:HB3	1:D:152:ALA:CB	2.41	0.50
1:F:162:LEU:HD21	1:F:180:ALA:HB3	1.93	0.50
1:B:703:ASN:C	1:B:703:ASN:HD22	2.19	0.50
1:B:867:ASN:HD22	1:B:867:ASN:N	2.09	0.50
1:B:983:ILE:HD12	1:B:983:ILE:N	2.27	0.50
1:E:278:LEU:HD23	1:E:287:PHE:HB3	1.93	0.50
1:A:568:LEU:HB3	1:A:571:MET:CE	2.41	0.50
1:C:48:ILE:HB	1:C:286:LEU:HD22	1.93	0.50
1:C:82:ASN:HD22	1:C:82:ASN:N	2.08	0.50
1:C:256:SER:OG	1:C:267:HIS:HE1	1.94	0.50
1:D:364:ILE:C	3:D:1325:HOH:O	2.54	0.50
1:E:365:ARG:HH21	1:E:365:ARG:HG2	1.75	0.50
1:E:710:ILE:HD13	1:E:713:ARG:HH22	1.77	0.50
1:F:82:ASN:HD21	1:F:96:ARG:HG2	1.76	0.50
1:F:558:SER:CB	3:F:1249:HOH:O	2.59	0.50
1:F:935:TYR:HB3	3:F:1254:HOH:O	2.11	0.50
1:F:1031:VAL:HG12	1:F:1033:ILE:CD1	2.42	0.50
1:A:887:MET:O	1:A:920:VAL:HG22	2.12	0.50
1:B:87:PHE:HB3	1:B:88:PRO:CD	2.39	0.50
1:B:480:ILE:HB	1:B:493:ALA:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:930:ASN:HD21	1:D:926:GLU:HG3	1.77	0.50
1:C:993:GLY:H	2:C:1214:DKT:HE11	1.77	0.50
1:F:185:PHE:HD2	3:F:1280:HOH:O	1.94	0.50
1:F:774:ASP:HA	1:F:817:ALA:HB2	1.94	0.50
1:C:858:ILE:HG13	3:C:1275:HOH:O	2.11	0.49
1:D:480:ILE:HB	1:D:493:ALA:HB3	1.93	0.49
1:D:489:LYS:HG3	1:D:491:PHE:CE1	2.47	0.49
1:D:578:ILE:O	1:D:578:ILE:HG13	2.11	0.49
1:E:489:LYS:HG3	1:E:491:PHE:CE1	2.47	0.49
1:F:381:THR:HA	3:F:1251:HOH:O	2.12	0.49
1:A:430:THR:O	3:A:1249:HOH:O	2.20	0.49
1:A:603:HIS:HD2	1:A:604:GLY:O	1.95	0.49
1:D:906:GLN:HG3	3:D:1302:HOH:O	2.11	0.49
1:F:578:ILE:O	1:F:578:ILE:HG13	2.11	0.49
1:A:498:SER:OG	1:A:518:ARG:HG2	2.12	0.49
1:B:175:LEU:O	1:B:177:LEU:HG	2.12	0.49
1:C:307:GLU:N	3:C:1304:HOH:O	2.29	0.49
1:C:645:ARG:HG3	1:C:645:ARG:NH2	2.27	0.49
1:E:444:SER:OG	1:E:466:PRO:HG2	2.12	0.49
1:E:541:VAL:HG22	1:E:542:ILE:N	2.27	0.49
1:F:82:ASN:HD21	1:F:96:ARG:HH21	1.60	0.49
1:F:460:PHE:CE2	1:F:568:LEU:HD11	2.47	0.49
1:A:362:LEU:HD13	1:A:688:GLN:HG3	1.95	0.49
1:B:534:GLU:OE1	3:B:1262:HOH:O	2.20	0.49
1:C:204:GLY:O	1:C:206:ARG:HG3	2.11	0.49
1:C:765:ILE:HD11	1:C:769:PHE:CZ	2.47	0.49
1:D:53:ILE:HG23	1:D:286:LEU:CD2	2.39	0.49
1:E:87:PHE:CB	1:E:88:PRO:HD2	2.40	0.49
1:E:568:LEU:HB3	1:E:571:MET:CE	2.38	0.49
1:F:57:CYS:HB3	1:F:62:TRP:NE1	2.28	0.49
1:A:645:ARG:HH21	1:A:645:ARG:HG3	1.77	0.49
1:C:1031:VAL:HG12	1:C:1033:ILE:CD1	2.42	0.49
1:F:164:ARG:NH2	1:F:166:GLU:OE1	2.46	0.49
1:F:225:ILE:O	1:F:261:GLY:HA3	2.12	0.49
1:F:578:ILE:HD11	1:F:580:VAL:CG2	2.38	0.49
1:D:99:ARG:N	3:D:1297:HOH:O	2.45	0.49
1:D:238:VAL:HG11	1:D:298:PRO:HG2	1.93	0.49
1:D:360:GLU:OE2	1:D:361:PRO:HD2	2.12	0.49
1:D:591:LEU:HD11	1:D:662:LEU:HD21	1.94	0.49
1:E:501:TYR:N	1:E:501:TYR:CD2	2.80	0.49
1:F:499:HIS:HD2	3:F:1263:HOH:O	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:HG2	1:A:365:ARG:HH21	1.78	0.49
1:A:642:SER:HB3	1:A:647:THR:HB	1.94	0.49
1:D:498:SER:OG	1:D:518:ARG:HG2	2.13	0.49
1:D:710:ILE:HD13	1:D:713:ARG:HH22	1.76	0.49
1:E:736:VAL:HG13	3:E:1276:HOH:O	2.11	0.49
1:F:802:PRO:O	1:F:805:TYR:HB2	2.13	0.49
1:C:222:PHE:H	1:C:1038:HIS:CD2	2.31	0.49
1:C:913:ARG:HH21	1:C:1047:GLN:NE2	2.11	0.49
1:E:104:ASN:ND2	3:E:1220:HOH:O	2.46	0.49
1:E:764:ARG:HG2	1:E:764:ARG:HH21	1.78	0.49
1:A:993:GLY:H	2:A:1214:DKT:HE11	1.76	0.49
1:C:87:PHE:CB	1:C:88:PRO:HD2	2.43	0.49
1:C:173:VAL:CB	3:C:1219:HOH:O	2.51	0.49
1:C:591:LEU:HD11	1:C:662:LEU:HD21	1.95	0.49
1:D:184:LEU:HD13	1:D:237:ILE:HG13	1.94	0.49
1:E:965:SER:HB3	2:E:1214:DKT:O	2.11	0.49
1:F:40:PRO:HG2	1:F:724:LEU:CD2	2.40	0.49
1:A:88:PRO:HG2	1:A:89:ASP:H	1.78	0.49
1:A:331:PRO:HD2	3:A:1226:HOH:O	2.12	0.49
1:A:480:ILE:HB	1:A:493:ALA:HB3	1.95	0.49
1:B:555:VAL:HG22	1:D:354:TYR:OH	2.12	0.49
1:B:591:LEU:HD11	1:B:662:LEU:HD21	1.94	0.49
1:B:993:GLY:H	2:B:1214:DKT:HE11	1.77	0.49
1:B:204:GLY:O	1:B:206:ARG:HG3	2.13	0.48
1:B:498:SER:OG	1:B:518:ARG:HG2	2.13	0.48
1:B:588:ILE:C	1:B:588:ILE:HD13	2.38	0.48
1:D:802:PRO:O	1:D:805:TYR:HB2	2.12	0.48
1:E:480:ILE:HB	1:E:493:ALA:HB3	1.95	0.48
1:E:837:LEU:HB2	1:E:845:ARG:HB2	1.95	0.48
1:C:559:MET:HG3	3:C:1220:HOH:O	2.13	0.48
1:C:867:ASN:HD22	1:C:867:ASN:N	2.11	0.48
1:C:889:MET:SD	1:D:522:PRO:HG2	2.53	0.48
1:F:429:MET:HG3	3:F:1276:HOH:O	2.13	0.48
1:D:541:VAL:HG22	1:D:542:ILE:N	2.28	0.48
1:E:550:ASN:C	1:E:550:ASN:OD1	2.56	0.48
1:F:87:PHE:CB	1:F:88:PRO:HD2	2.42	0.48
1:B:124:PHE:HB3	1:B:152:ALA:CB	2.42	0.48
1:B:645:ARG:NH2	1:B:645:ARG:HG3	2.28	0.48
1:B:909:ILE:HG12	1:B:956:ILE:CG2	2.44	0.48
1:C:460:PHE:CE2	1:C:568:LEU:HD11	2.49	0.48
1:C:940:ARG:HD3	1:D:424:ASP:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:913:ARG:HH21	1:F:1047:GLN:NE2	2.10	0.48
1:B:501:TYR:N	1:B:501:TYR:CD2	2.81	0.48
1:D:322:PRO:HG3	1:D:673:THR:O	2.14	0.48
1:E:57:CYS:HB3	1:E:62:TRP:NE1	2.27	0.48
1:F:489:LYS:HG3	1:F:491:PHE:CE1	2.48	0.48
1:F:959:THR:O	1:F:984:GLY:HA3	2.13	0.48
1:F:988:TRP:CG	3:F:1256:HOH:O	2.66	0.48
1:A:639:LEU:HD23	1:A:640:ARG:N	2.28	0.48
1:A:645:ARG:HG3	1:A:645:ARG:NH2	2.28	0.48
1:B:238:VAL:HG11	1:B:298:PRO:HG2	1.94	0.48
1:B:645:ARG:HG3	1:B:645:ARG:HH21	1.78	0.48
1:F:467:LEU:C	1:F:467:LEU:HD12	2.38	0.48
1:F:498:SER:OG	1:F:518:ARG:HG2	2.13	0.48
1:B:293:ILE:HG22	1:B:306:ILE:HD12	1.95	0.48
1:C:319:ILE:HG23	1:C:677:PRO:HB3	1.96	0.48
1:C:728:ARG:HG3	1:C:754:PHE:CE1	2.49	0.48
1:D:642:SER:HB3	1:D:647:THR:HB	1.95	0.48
1:D:993:GLY:H	2:D:1214:DKT:HE11	1.78	0.48
1:D:1031:VAL:HG12	1:D:1033:ILE:CD1	2.44	0.48
1:F:200:PRO:O	1:F:740:GLY:HA3	2.14	0.48
1:F:431:VAL:HG22	3:F:1276:HOH:O	2.12	0.48
1:C:154:GLN:HG2	3:C:1323:HOH:O	2.12	0.48
1:C:524:PRO:HD3	1:D:605:GLU:CG	2.43	0.48
1:C:975:LYS:HA	3:C:1265:HOH:O	2.14	0.48
1:D:887:MET:O	1:D:920:VAL:HG22	2.13	0.48
1:E:588:ILE:C	1:E:588:ILE:HD13	2.39	0.48
1:F:336:LEU:O	1:F:337:ILE:HD13	2.14	0.48
1:F:362:LEU:HD13	1:F:688:GLN:HG3	1.96	0.48
1:A:406:ASN:HD22	1:A:424:ASP:CG	2.22	0.48
1:A:605:GLU:HG2	1:B:524:PRO:HD3	1.94	0.48
1:A:710:ILE:HD13	1:A:713:ARG:HH22	1.78	0.48
1:A:965:SER:HB2	2:A:1214:DKT:C6	2.38	0.48
1:B:336:LEU:O	1:B:337:ILE:HD13	2.13	0.48
1:B:837:LEU:HB2	1:B:845:ARG:HB2	1.96	0.48
1:C:791:GLU:CD	1:C:861:ARG:HE	2.22	0.48
1:C:1011:PHE:HB3	1:D:936:ASP:OD2	2.12	0.48
1:F:406:ASN:HD22	1:F:424:ASP:CG	2.21	0.48
1:C:64:HIS:HB2	1:C:71:THR:HG23	1.96	0.48
1:C:87:PHE:HB3	1:C:88:PRO:CD	2.43	0.48
1:C:588:ILE:HD13	1:C:588:ILE:C	2.38	0.48
1:C:703:ASN:OD1	1:C:706:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:545:ILE:HD12	1:D:545:ILE:N	2.28	0.48
1:D:546:PRO:HG2	1:D:567:ASP:HB3	1.95	0.48
1:E:184:LEU:HD13	1:E:237:ILE:HG13	1.96	0.48
1:E:285:ILE:HD12	1:E:296:PHE:HD2	1.79	0.48
1:E:347:ILE:HG12	1:E:392:TYR:CD2	2.49	0.48
1:E:498:SER:OG	1:E:518:ARG:HG2	2.14	0.48
1:E:524:PRO:HD3	1:F:605:GLU:CG	2.44	0.48
1:F:87:PHE:HB3	1:F:88:PRO:CD	2.43	0.48
1:F:913:ARG:O	1:F:914:PHE:HB2	2.13	0.48
1:F:993:GLY:H	2:F:1214:DKT:HE11	1.78	0.48
1:A:501:TYR:CD2	1:A:501:TYR:N	2.81	0.47
1:A:986:ARG:HA	1:A:1027:VAL:O	2.14	0.47
1:C:82:ASN:HD21	1:C:96:ARG:HG2	1.79	0.47
1:C:225:ILE:O	1:C:261:GLY:HA3	2.13	0.47
1:E:367:VAL:CG1	1:E:375:VAL:HG21	2.44	0.47
1:E:545:ILE:HD12	1:E:545:ILE:N	2.29	0.47
1:A:1010:GLU:HB3	1:A:1011:PHE:CE1	2.49	0.47
1:B:88:PRO:HG2	1:B:89:ASP:H	1.79	0.47
1:B:143:ASP:CG	3:B:1287:HOH:O	2.57	0.47
1:E:322:PRO:HG2	1:E:674:ASP:OD1	2.14	0.47
1:E:530:ASN:HD22	1:E:531:PHE:N	2.06	0.47
1:F:138:ALA:HB3	3:F:1293:HOH:O	2.13	0.47
1:F:591:LEU:HD11	1:F:662:LEU:HD21	1.95	0.47
1:F:765:ILE:HD11	1:F:769:PHE:HZ	1.79	0.47
1:F:1009:PRO:HB3	3:F:1257:HOH:O	2.14	0.47
1:C:462:ALA:HA	1:C:481:HIS:O	2.13	0.47
1:C:983:ILE:HD12	1:C:983:ILE:N	2.29	0.47
1:D:131:ARG:HG2	1:D:131:ARG:HH21	1.79	0.47
1:D:501:TYR:CD2	1:D:501:TYR:N	2.82	0.47
1:D:837:LEU:HB2	1:D:845:ARG:HB2	1.96	0.47
1:E:53:ILE:CG2	1:E:286:LEU:HD21	2.42	0.47
1:E:638:ASP:HB3	1:E:651:ARG:HB3	1.97	0.47
1:F:48:ILE:CG2	3:F:1265:HOH:O	2.62	0.47
1:F:765:ILE:HD11	1:F:769:PHE:CZ	2.48	0.47
1:F:989:GLY:C	3:F:1256:HOH:O	2.56	0.47
1:A:322:PRO:HG3	1:A:673:THR:O	2.14	0.47
1:A:336:LEU:O	1:A:337:ILE:HD13	2.13	0.47
1:A:578:ILE:HD11	1:A:580:VAL:CG2	2.41	0.47
1:E:605:GLU:CG	1:F:524:PRO:HD3	2.45	0.47
1:E:1010:GLU:HB3	1:E:1011:PHE:CE1	2.50	0.47
1:A:837:LEU:HB2	1:A:845:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:LEU:HD22	1:C:55:PHE:CE1	2.50	0.47
1:C:336:LEU:O	1:C:337:ILE:HD13	2.15	0.47
1:D:87:PHE:HB3	1:D:88:PRO:CD	2.43	0.47
1:D:550:ASN:C	1:D:550:ASN:OD1	2.56	0.47
1:E:53:ILE:HG23	1:E:286:LEU:CD2	2.41	0.47
1:E:993:GLY:H	2:E:1214:DKT:HE11	1.79	0.47
1:F:703:ASN:OD1	1:F:706:VAL:HG23	2.14	0.47
1:F:983:ILE:HD12	1:F:983:ILE:N	2.29	0.47
1:A:53:ILE:HG23	1:A:286:LEU:CD2	2.42	0.47
1:A:591:LEU:HD11	1:A:662:LEU:HD21	1.96	0.47
1:B:791:GLU:CD	1:B:861:ARG:HE	2.22	0.47
1:C:57:CYS:HB3	1:C:62:TRP:NE1	2.28	0.47
1:C:393:ARG:NH1	1:E:558:SER:HA	2.30	0.47
1:C:605:GLU:CG	1:D:524:PRO:HD3	2.45	0.47
1:D:515:LEU:HD23	1:D:539:PRO:HA	1.96	0.47
1:D:872:HIS:HE1	1:D:902:GLU:OE1	1.97	0.47
1:E:515:LEU:HD23	1:E:539:PRO:HA	1.97	0.47
1:F:799:GLY:O	1:F:800:ILE:HG23	2.14	0.47
1:F:887:MET:O	1:F:920:VAL:HG22	2.15	0.47
1:A:82:ASN:HD22	1:A:82:ASN:N	2.11	0.47
1:A:87:PHE:CB	1:A:88:PRO:HD2	2.42	0.47
1:A:164:ARG:NH2	1:A:166:GLU:OE1	2.48	0.47
1:A:604:GLY:HA3	1:B:521:ASP:CG	2.40	0.47
1:A:694:TRP:HA	1:A:738:MET:CE	2.45	0.47
1:B:284:ARG:NE	3:B:1320:HOH:O	2.46	0.47
1:B:1032:GLU:C	1:B:1033:ILE:HD12	2.39	0.47
1:C:489:LYS:HG3	1:C:491:PHE:CE1	2.49	0.47
1:C:789:GLU:CB	3:D:1308:HOH:O	2.63	0.47
1:D:131:ARG:HH12	2:D:1214:DKT:CD6	2.27	0.47
1:D:256:SER:OG	1:D:267:HIS:HE1	1.97	0.47
1:D:322:PRO:HG2	1:D:674:ASP:OD1	2.13	0.47
1:D:638:ASP:HB3	1:D:651:ARG:HB3	1.96	0.47
1:E:867:ASN:HD22	1:E:867:ASN:N	2.13	0.47
1:F:579:ASN:HA	3:F:1264:HOH:O	2.14	0.47
1:A:124:PHE:HB3	1:A:152:ALA:CB	2.45	0.47
1:A:703:ASN:OD1	1:A:706:VAL:HG23	2.14	0.47
1:A:799:GLY:O	1:A:800:ILE:HG23	2.14	0.47
1:B:545:ILE:HD12	1:B:545:ILE:N	2.29	0.47
1:C:734:VAL:HG12	3:C:1306:HOH:O	2.13	0.47
1:D:603:HIS:HD2	1:D:604:GLY:O	1.98	0.47
1:D:897:ARG:CZ	3:D:1267:HOH:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:LEU:HD21	1:E:180:ALA:HB3	1.97	0.47
1:E:204:GLY:O	1:E:206:ARG:HG3	2.15	0.47
1:F:319:ILE:HG23	1:F:677:PRO:HB3	1.96	0.47
1:F:438:PRO:HA	3:F:1276:HOH:O	2.15	0.47
1:F:467:LEU:N	3:F:1283:HOH:O	2.47	0.47
1:F:588:ILE:HD13	1:F:588:ILE:C	2.39	0.47
1:F:638:ASP:HB3	1:F:651:ARG:HB3	1.96	0.47
1:A:57:CYS:HB3	1:A:62:TRP:CD1	2.50	0.47
1:A:225:ILE:O	1:A:261:GLY:HA3	2.14	0.47
1:A:342:ARG:O	3:A:1241:HOH:O	2.20	0.47
1:A:936:ASP:HB3	1:A:944:SER:HB3	1.97	0.47
1:C:1032:GLU:C	1:C:1033:ILE:HD12	2.40	0.47
1:D:598:TYR:HE1	3:D:1310:HOH:O	1.96	0.47
1:B:460:PHE:CE2	1:B:568:LEU:HD11	2.50	0.47
1:C:146:LEU:HD23	1:C:165:VAL:HG21	1.96	0.47
1:C:155:PRO:HG2	1:C:156:PHE:CD1	2.50	0.47
1:C:200:PRO:O	1:C:740:GLY:HA3	2.15	0.47
1:D:57:CYS:HB3	1:D:62:TRP:NE1	2.30	0.47
1:E:293:ILE:HG22	1:E:306:ILE:HD12	1.96	0.47
1:E:406:ASN:HD22	1:E:424:ASP:CG	2.22	0.47
1:E:885:PRO:O	1:E:915:ASN:HA	2.15	0.47
1:F:986:ARG:HA	1:F:1027:VAL:O	2.15	0.47
1:A:353:THR:HG23	1:A:354:TYR:CD1	2.50	0.46
1:B:444:SER:OG	1:B:466:PRO:HG2	2.16	0.46
1:C:53:ILE:HG23	1:C:286:LEU:CD2	2.44	0.46
1:C:521:ASP:OD1	1:D:604:GLY:HA3	2.16	0.46
1:D:588:ILE:C	1:D:588:ILE:HD13	2.39	0.46
1:E:243:TYR:CD2	1:E:256:SER:HB3	2.50	0.46
1:E:546:PRO:CG	1:E:567:ASP:HB3	2.45	0.46
1:E:936:ASP:OD2	1:F:1011:PHE:HB3	2.15	0.46
1:A:64:HIS:HB2	1:A:71:THR:HG23	1.97	0.46
1:B:322:PRO:HG2	1:B:674:ASP:OD1	2.14	0.46
1:B:799:GLY:O	1:B:800:ILE:HG23	2.16	0.46
1:C:473:ASP:HA	1:D:904:SER:CB	2.45	0.46
1:C:765:ILE:HD11	1:C:769:PHE:HZ	1.80	0.46
1:C:913:ARG:O	1:C:914:PHE:HB2	2.15	0.46
1:D:365:ARG:HG2	1:D:365:ARG:HH21	1.80	0.46
1:D:442:GLU:OE2	1:D:481:HIS:HD2	1.99	0.46
1:E:128:SER:OG	3:E:1230:HOH:O	1.97	0.46
1:F:545:ILE:N	1:F:545:ILE:HD12	2.30	0.46
1:F:710:ILE:HD13	1:F:713:ARG:NH2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:768:ASP:HB2	1:F:780:LYS:HB3	1.97	0.46
1:A:222:PHE:H	1:A:1038:HIS:CD2	2.34	0.46
1:A:802:PRO:O	1:A:805:TYR:HB2	2.16	0.46
1:B:45:ASN:HB3	1:B:277:HIS:CE1	2.51	0.46
1:B:49:HIS:CD2	3:B:1225:HOH:O	2.67	0.46
1:B:93:ILE:HD12	1:B:111:TYR:HD2	1.80	0.46
1:C:562:GLU:C	1:C:564:GLY:H	2.23	0.46
1:C:869:ARG:NH2	3:C:1310:HOH:O	2.48	0.46
1:D:82:ASN:ND2	1:D:96:ARG:HH21	2.13	0.46
1:D:1010:GLU:HB3	1:D:1011:PHE:CE1	2.50	0.46
1:E:57:CYS:HB3	1:E:62:TRP:CD1	2.50	0.46
1:F:204:GLY:O	1:F:206:ARG:HG3	2.15	0.46
1:A:87:PHE:HB3	1:A:88:PRO:CD	2.45	0.46
1:B:64:HIS:HB2	1:B:71:THR:HG23	1.96	0.46
1:C:406:ASN:HD22	1:C:424:ASP:CG	2.23	0.46
1:C:618:VAL:CG2	1:C:631:GLU:HG3	2.45	0.46
1:C:771:LEU:CA	3:C:1234:HOH:O	2.62	0.46
1:E:88:PRO:CB	3:E:1234:HOH:O	2.52	0.46
1:E:703:ASN:C	1:E:703:ASN:ND2	2.73	0.46
1:A:57:CYS:HB3	1:A:62:TRP:NE1	2.31	0.46
1:C:141:ASP:C	1:C:141:ASP:OD2	2.58	0.46
1:C:603:HIS:HD2	1:C:604:GLY:O	1.98	0.46
1:D:243:TYR:CD2	1:D:256:SER:HB3	2.51	0.46
1:D:994:ILE:O	1:D:994:ILE:HD12	2.16	0.46
1:E:82:ASN:HD21	1:E:96:ARG:HG2	1.80	0.46
1:B:765:ILE:HD11	1:B:769:PHE:CZ	2.51	0.46
1:C:180:ALA:CA	3:C:1311:HOH:O	2.63	0.46
1:C:550:ASN:C	1:C:550:ASN:OD1	2.58	0.46
1:C:676:ARG:HG2	3:C:1236:HOH:O	2.15	0.46
1:C:710:ILE:HD13	1:C:713:ARG:NH2	2.30	0.46
1:D:53:ILE:CG2	1:D:286:LEU:HD21	2.43	0.46
1:D:406:ASN:HD22	1:D:424:ASP:CG	2.23	0.46
1:E:131:ARG:HH12	2:E:1214:DKT:CD6	2.29	0.46
1:F:546:PRO:HG2	1:F:567:ASP:HB3	1.97	0.46
1:F:770:LYS:O	1:F:777:VAL:HG12	2.16	0.46
1:B:642:SER:HB3	1:B:647:THR:HB	1.96	0.46
1:C:788:ASN:ND2	3:C:1338:HOH:O	2.37	0.46
1:D:200:PRO:O	1:D:740:GLY:HA3	2.16	0.46
1:D:460:PHE:CE2	1:D:568:LEU:HD11	2.50	0.46
1:E:442:GLU:OE2	1:E:481:HIS:HD2	1.99	0.46
1:F:462:ALA:HA	1:F:481:HIS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:768:ASP:HB2	1:C:780:LYS:HB3	1.98	0.46
1:C:960:ASN:N	3:C:1247:HOH:O	2.48	0.46
1:D:285:ILE:HD12	1:D:296:PHE:HD2	1.81	0.46
1:D:1032:GLU:C	1:D:1033:ILE:HD12	2.41	0.46
1:E:497:ASN:HB2	3:E:1278:HOH:O	2.16	0.46
1:F:64:HIS:HB2	1:F:71:THR:HG23	1.98	0.46
1:F:381:THR:CA	3:F:1251:HOH:O	2.63	0.46
1:F:687:LEU:HD23	1:F:722:VAL:HG11	1.97	0.46
1:F:744:THR:HG22	1:F:745:SER:H	1.80	0.46
1:A:765:ILE:HD11	1:A:769:PHE:CZ	2.51	0.46
1:A:909:ILE:HG12	1:A:956:ILE:CG2	2.46	0.46
1:C:789:GLU:HB2	3:D:1308:HOH:O	2.16	0.46
1:C:887:MET:HB2	1:C:917:GLY:C	2.41	0.46
1:D:40:PRO:HG2	1:D:724:LEU:CD2	2.40	0.46
1:D:293:ILE:HG22	1:D:306:ILE:HD12	1.98	0.46
1:A:983:ILE:HD12	1:A:983:ILE:N	2.30	0.46
1:B:319:ILE:HG23	1:B:677:PRO:HB3	1.98	0.46
1:B:550:ASN:C	1:B:550:ASN:OD1	2.59	0.46
1:C:390:TYR:HD1	1:C:397:ALA:HB2	1.81	0.46
1:C:546:PRO:HG2	1:C:567:ASP:HB3	1.98	0.46
1:E:272:ASP:OD1	1:E:289:LYS:NZ	2.49	0.46
1:E:351:SER:OG	1:E:353:THR:CG2	2.63	0.46
1:B:578:ILE:HD11	1:B:580:VAL:CG2	2.41	0.45
1:C:346:PHE:CD1	3:C:1298:HOH:O	2.56	0.45
1:C:424:ASP:O	1:D:940:ARG:HD3	2.16	0.45
1:D:558:SER:HA	1:F:393:ARG:NH1	2.31	0.45
1:F:867:ASN:HD22	1:F:867:ASN:N	2.14	0.45
1:A:541:VAL:HG22	1:A:542:ILE:N	2.31	0.45
1:A:545:ILE:HD12	1:A:545:ILE:N	2.32	0.45
1:B:313:SER:O	1:E:117:GLU:HA	2.15	0.45
1:B:823:ARG:HD2	1:E:317:ARG:HD3	1.98	0.45
1:C:118:ILE:HG22	1:F:314:PRO:HA	1.98	0.45
1:C:714:ILE:HG21	1:C:741:GLU:HB3	1.97	0.45
1:D:367:VAL:CG1	1:D:375:VAL:HG21	2.45	0.45
1:E:300:THR:HG22	1:E:302:LYS:HB2	1.98	0.45
1:F:348:GLN:HB3	3:F:1299:HOH:O	2.16	0.45
1:F:367:VAL:CG1	1:F:375:VAL:HG21	2.46	0.45
1:F:518:ARG:C	3:F:1221:HOH:O	2.59	0.45
1:A:131:ARG:HG2	1:A:131:ARG:HH21	1.81	0.45
1:A:765:ILE:HD11	1:A:769:PHE:HZ	1.81	0.45
1:A:913:ARG:HH21	1:A:1047:GLN:NE2	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:LEU:HD13	1:B:688:GLN:HG3	1.97	0.45
1:B:1014:TRP:CD1	1:B:1019:GLY:HA2	2.50	0.45
1:B:1014:TRP:NE1	1:B:1019:GLY:HA2	2.31	0.45
1:C:45:ASN:HA	1:C:277:HIS:CG	2.51	0.45
1:D:82:ASN:HD21	1:D:96:ARG:HG2	1.79	0.45
1:D:706:VAL:HG12	1:D:710:ILE:HG12	1.98	0.45
1:F:285:ILE:HD12	1:F:296:PHE:HD2	1.80	0.45
1:F:599:SER:CA	3:F:1302:HOH:O	2.63	0.45
1:F:890:MET:O	1:F:894:GLU:HG2	2.16	0.45
1:D:171:ASN:HB2	1:D:771:LEU:HB2	1.98	0.45
1:D:300:THR:HG22	1:D:302:LYS:HB2	1.97	0.45
1:D:703:ASN:C	1:D:703:ASN:ND2	2.72	0.45
1:D:909:ILE:HG12	1:D:956:ILE:CG2	2.46	0.45
1:E:913:ARG:HH21	1:E:1047:GLN:NE2	2.12	0.45
1:F:88:PRO:HG2	1:F:89:ASP:H	1.81	0.45
1:F:515:LEU:HD23	1:F:539:PRO:HA	1.99	0.45
1:F:684:GLU:HG3	1:F:685:GLU:N	2.32	0.45
1:A:190:ARG:HB3	3:A:1266:HOH:O	2.15	0.45
1:B:57:CYS:HB3	1:B:62:TRP:NE1	2.30	0.45
1:B:222:PHE:H	1:B:1038:HIS:CD2	2.35	0.45
1:B:694:TRP:HA	1:B:738:MET:CE	2.47	0.45
1:C:618:VAL:HG21	1:C:631:GLU:HG3	1.98	0.45
1:D:362:LEU:HD13	1:D:688:GLN:HG3	1.97	0.45
1:D:983:ILE:HD12	1:D:983:ILE:N	2.29	0.45
1:E:746:HIS:HA	1:E:748:TYR:CE2	2.51	0.45
1:E:889:MET:SD	1:F:522:PRO:HG2	2.56	0.45
1:F:57:CYS:HB3	1:F:62:TRP:CD1	2.51	0.45
1:A:546:PRO:HG2	1:A:567:ASP:HB3	1.98	0.45
1:B:45:ASN:HA	1:B:277:HIS:CG	2.51	0.45
1:C:57:CYS:HB3	1:C:62:TRP:CD1	2.51	0.45
1:C:347:ILE:HG12	1:C:392:TYR:CD2	2.52	0.45
1:C:887:MET:O	1:C:920:VAL:HG22	2.17	0.45
1:D:467:LEU:C	1:D:467:LEU:HD12	2.41	0.45
1:F:442:GLU:OE2	1:F:481:HIS:HD2	1.99	0.45
1:A:243:TYR:CD2	1:A:256:SER:HB3	2.52	0.45
1:A:603:HIS:CD2	1:A:604:GLY:O	2.70	0.45
1:A:744:THR:HG22	1:A:745:SER:H	1.80	0.45
1:C:243:TYR:CD2	1:C:256:SER:HB3	2.52	0.45
1:C:317:ARG:CD	1:F:823:ARG:HD2	2.43	0.45
1:D:728:ARG:HG3	1:D:754:PHE:CE1	2.50	0.45
1:D:894:GLU:OE2	1:D:894:GLU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:TYR:HD1	1:F:397:ALA:HB2	1.81	0.45
1:F:1010:GLU:HB3	1:F:1011:PHE:CE1	2.52	0.45
1:A:45:ASN:HA	1:A:277:HIS:CG	2.52	0.45
1:B:57:CYS:HB3	1:B:62:TRP:CD1	2.51	0.45
1:B:347:ILE:HG12	1:B:392:TYR:CD2	2.52	0.45
1:B:887:MET:O	1:B:920:VAL:HG22	2.16	0.45
1:C:46:PRO:HB2	1:C:286:LEU:CD2	2.46	0.45
1:C:522:PRO:CG	1:D:889:MET:SD	3.05	0.45
1:C:638:ASP:HB3	1:C:651:ARG:HB3	1.99	0.45
1:C:936:ASP:HB3	1:C:944:SER:HB3	1.99	0.45
1:D:279:ASN:HD22	1:D:279:ASN:HA	1.58	0.45
1:D:444:SER:OG	1:D:466:PRO:HG2	2.17	0.45
1:D:739:GLN:NE2	3:D:1229:HOH:O	2.49	0.45
1:E:82:ASN:ND2	1:E:96:ARG:HH21	2.14	0.45
1:E:460:PHE:CE2	1:E:568:LEU:HD11	2.52	0.45
1:E:524:PRO:HD3	1:F:605:GLU:HG2	1.99	0.45
1:E:707:ALA:HB2	3:F:1216:HOH:O	2.16	0.45
1:F:45:ASN:HA	1:F:277:HIS:CG	2.52	0.45
1:F:228:MET:HE1	1:F:244:PHE:CE1	2.52	0.45
1:F:694:TRP:HA	1:F:738:MET:CE	2.47	0.45
1:F:714:ILE:HG21	1:F:741:GLU:HG3	1.99	0.45
1:F:894:GLU:HA	1:F:894:GLU:OE2	2.17	0.45
1:A:253:GLN:NE2	1:A:270:PHE:H	2.05	0.45
1:A:319:ILE:HG23	1:A:677:PRO:HB3	1.98	0.45
1:A:714:ILE:HG21	1:A:741:GLU:HB3	1.99	0.45
1:B:467:LEU:C	1:B:467:LEU:HD12	2.41	0.45
1:B:710:ILE:HD13	1:B:713:ARG:NH2	2.32	0.45
1:B:874:ARG:HH11	1:B:1053:ASP:CG	2.24	0.45
1:B:925:ILE:HB	3:B:1243:HOH:O	2.17	0.45
1:B:1010:GLU:HB3	1:B:1011:PHE:CE1	2.52	0.45
1:C:351:SER:CB	1:C:353:THR:HG22	2.45	0.45
1:D:347:ILE:HG12	1:D:392:TYR:CD2	2.51	0.45
1:D:363:ARG:HD3	1:D:363:ARG:HA	1.76	0.45
1:D:639:LEU:HD23	1:D:640:ARG:N	2.32	0.45
1:E:285:ILE:HD12	1:E:296:PHE:CD2	2.52	0.45
1:E:874:ARG:HH11	1:E:1053:ASP:CG	2.24	0.45
1:E:890:MET:O	1:E:894:GLU:HG2	2.16	0.45
1:E:909:ILE:HG12	1:E:956:ILE:CG2	2.47	0.45
1:A:155:PRO:HG2	1:A:156:PHE:CD1	2.52	0.45
1:B:728:ARG:HG3	1:B:754:PHE:CE1	2.52	0.45
1:C:88:PRO:HG2	1:C:89:ASP:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:PHE:HB3	1:C:536:VAL:HG11	1.99	0.45
1:C:986:ARG:HA	1:C:1027:VAL:O	2.17	0.45
1:D:746:HIS:HA	1:D:748:TYR:CE2	2.52	0.45
1:F:125:SER:CB	1:F:762:SER:HB2	2.47	0.45
1:F:285:ILE:HD12	1:F:296:PHE:CD2	2.52	0.45
1:F:568:LEU:HB3	1:F:571:MET:CE	2.45	0.45
1:A:145:ASN:CB	3:A:1264:HOH:O	2.65	0.44
1:B:714:ILE:HG21	1:B:741:GLU:HB3	2.00	0.44
1:C:218:ASN:HB3	1:C:221:ALA:HB3	1.98	0.44
1:C:966:ASP:HA	3:C:1276:HOH:O	2.16	0.44
1:F:320:SER:HA	3:F:1218:HOH:O	2.17	0.44
1:A:200:PRO:O	1:A:740:GLY:HA3	2.17	0.44
1:A:293:ILE:HG22	1:A:306:ILE:HD12	1.98	0.44
1:A:467:LEU:HD12	1:A:467:LEU:C	2.43	0.44
1:A:1032:GLU:C	1:A:1033:ILE:HD12	2.42	0.44
1:B:285:ILE:HD12	1:B:296:PHE:HD2	1.83	0.44
1:C:694:TRP:HA	1:C:738:MET:CE	2.48	0.44
1:D:809:ASP:HB3	1:D:814:THR:HA	1.99	0.44
1:E:442:GLU:CG	3:E:1242:HOH:O	2.63	0.44
1:E:942:THR:OG1	1:F:468:LYS:CE	2.65	0.44
1:E:983:ILE:HD12	1:E:983:ILE:N	2.32	0.44
1:F:501:TYR:CD2	1:F:501:TYR:N	2.85	0.44
1:B:225:ILE:O	1:B:261:GLY:HA3	2.17	0.44
1:B:684:GLU:HG3	1:B:685:GLU:N	2.32	0.44
1:D:204:GLY:O	1:D:206:ARG:HG3	2.18	0.44
1:E:467:LEU:C	1:E:467:LEU:HD12	2.43	0.44
1:A:467:LEU:HD21	1:A:496:GLU:HB3	1.99	0.44
1:B:141:ASP:OD2	1:B:141:ASP:C	2.61	0.44
1:B:322:PRO:HG3	1:B:673:THR:O	2.17	0.44
1:B:731:LEU:O	1:B:731:LEU:HD22	2.17	0.44
1:C:196:THR:CA	3:C:1274:HOH:O	2.62	0.44
1:D:218:ASN:C	3:D:1340:HOH:O	2.60	0.44
1:D:390:TYR:HD1	1:D:397:ALA:HB2	1.83	0.44
1:E:942:THR:OG1	1:F:468:LYS:HE2	2.17	0.44
1:E:993:GLY:N	1:E:1011:PHE:O	2.50	0.44
1:F:109:TYR:HD1	3:F:1217:HOH:O	2.01	0.44
1:F:1014:TRP:CD1	1:F:1019:GLY:HA2	2.53	0.44
1:A:322:PRO:HG2	1:A:674:ASP:OD1	2.17	0.44
1:B:406:ASN:HD22	1:B:424:ASP:CG	2.25	0.44
1:C:131:ARG:HG2	1:C:131:ARG:HH21	1.82	0.44
1:C:440:VAL:CG1	3:C:1267:HOH:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:604:GLY:HA3	1:D:521:ASP:OD1	2.18	0.44
1:D:885:PRO:O	1:D:915:ASN:HA	2.17	0.44
1:D:976:LYS:NZ	1:D:1017:ASP:HB2	2.32	0.44
1:E:45:ASN:HA	1:E:277:HIS:CG	2.53	0.44
1:E:91:ARG:NH1	1:E:114:GLU:HB2	2.32	0.44
1:E:359:PRO:HA	3:E:1251:HOH:O	2.16	0.44
1:E:1032:GLU:C	1:E:1033:ILE:HD12	2.43	0.44
1:F:243:TYR:CD2	1:F:256:SER:HB3	2.52	0.44
1:A:1014:TRP:CD1	1:A:1019:GLY:HA2	2.53	0.44
1:B:131:ARG:HH12	2:B:1214:DKT:CD6	2.31	0.44
1:C:99:ARG:HD2	1:C:760:PHE:CZ	2.52	0.44
1:C:285:ILE:HD12	1:C:296:PHE:HD2	1.82	0.44
1:C:603:HIS:CD2	1:C:604:GLY:O	2.71	0.44
1:C:1014:TRP:CD1	1:C:1019:GLY:HA2	2.53	0.44
1:D:131:ARG:HH12	2:D:1214:DKT:HD61	1.83	0.44
1:D:694:TRP:HA	1:D:738:MET:CE	2.47	0.44
1:F:703:ASN:C	1:F:703:ASN:ND2	2.75	0.44
1:A:639:LEU:HD23	1:A:639:LEU:C	2.42	0.44
1:C:279:ASN:HD22	1:C:279:ASN:HA	1.57	0.44
1:C:679:VAL:N	3:C:1291:HOH:O	2.50	0.44
1:C:746:HIS:HA	1:C:748:TYR:CE2	2.52	0.44
1:C:929:MET:HE3	1:C:979:LEU:CD1	2.47	0.44
1:D:43:LEU:HD22	1:D:55:PHE:CE1	2.53	0.44
1:D:57:CYS:HB3	1:D:62:TRP:CD1	2.52	0.44
1:D:87:PHE:CB	1:D:88:PRO:HD2	2.42	0.44
1:F:1032:GLU:C	1:F:1033:ILE:HD12	2.42	0.44
1:A:562:GLU:C	1:A:564:GLY:H	2.25	0.44
1:B:131:ARG:HH21	1:B:131:ARG:HG2	1.83	0.44
1:B:363:ARG:HA	1:B:363:ARG:HD3	1.76	0.44
1:B:393:ARG:CZ	1:F:558:SER:HA	2.48	0.44
1:B:462:ALA:HA	1:B:481:HIS:O	2.18	0.44
1:B:546:PRO:HG2	1:B:567:ASP:HB3	2.00	0.44
1:B:662:LEU:HD12	1:B:662:LEU:O	2.18	0.44
1:C:228:MET:HE1	1:C:244:PHE:CE1	2.53	0.44
1:D:45:ASN:HA	1:D:277:HIS:CG	2.53	0.44
1:F:162:LEU:HG	3:F:1295:HOH:O	2.18	0.44
1:F:322:PRO:HG3	1:F:673:THR:O	2.17	0.44
1:A:82:ASN:HD21	1:A:96:ARG:HH21	1.65	0.44
1:B:131:ARG:HA	3:B:1226:HOH:O	2.17	0.44
1:B:200:PRO:O	1:B:740:GLY:HA3	2.16	0.44
1:C:40:PRO:HG2	1:C:724:LEU:CD2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:PRO:HG2	1:C:674:ASP:OD1	2.17	0.44
1:C:764:ARG:HG2	1:C:764:ARG:HH21	1.83	0.44
1:D:618:VAL:CG2	1:D:631:GLU:HG3	2.48	0.44
1:D:913:ARG:HH21	1:D:1047:GLN:NE2	2.12	0.44
1:E:462:ALA:HA	1:E:481:HIS:O	2.17	0.44
1:F:46:PRO:HD3	1:F:288:SER:HB3	2.00	0.44
1:F:146:LEU:HD23	1:F:165:VAL:HG21	1.99	0.44
1:F:562:GLU:C	1:F:564:GLY:H	2.25	0.44
1:A:175:LEU:O	1:A:177:LEU:HG	2.18	0.43
1:A:728:ARG:HG3	1:A:754:PHE:CE1	2.53	0.43
1:A:809:ASP:HB3	1:A:814:THR:HA	2.00	0.43
1:A:1014:TRP:NE1	1:A:1019:GLY:HA2	2.33	0.43
1:B:228:MET:HE1	1:B:244:PHE:CE1	2.53	0.43
1:C:936:ASP:OD2	1:D:1011:PHE:HB3	2.17	0.43
1:D:131:ARG:NH1	2:D:1214:DKT:HD62	2.33	0.43
1:D:162:LEU:HD21	1:D:180:ALA:HB3	1.99	0.43
1:D:731:LEU:HD13	1:D:735:ILE:HD12	1.99	0.43
1:E:894:GLU:HA	1:E:894:GLU:OE2	2.17	0.43
1:E:1031:VAL:HG12	1:E:1033:ILE:HD12	1.99	0.43
1:F:272:ASP:OD1	1:F:289:LYS:NZ	2.51	0.43
1:A:350:VAL:HG23	1:A:351:SER:N	2.33	0.43
1:A:588:ILE:HD13	1:A:588:ILE:C	2.42	0.43
1:B:703:ASN:OD1	1:B:706:VAL:HG23	2.18	0.43
1:C:99:ARG:HD2	1:C:760:PHE:CE2	2.52	0.43
1:C:125:SER:CB	1:C:762:SER:HB2	2.48	0.43
1:C:131:ARG:HH12	2:C:1214:DKT:CD6	2.30	0.43
1:C:501:TYR:CD2	1:C:501:TYR:N	2.86	0.43
1:C:703:ASN:C	1:C:703:ASN:ND2	2.75	0.43
1:D:897:ARG:NH1	3:D:1267:HOH:O	2.50	0.43
1:E:141:ASP:C	1:E:141:ASP:OD2	2.60	0.43
1:F:322:PRO:HG2	1:F:674:ASP:OD1	2.18	0.43
1:F:444:SER:OG	1:F:466:PRO:HG2	2.18	0.43
1:A:45:ASN:HB3	1:A:277:HIS:CE1	2.54	0.43
1:A:146:LEU:HD23	1:A:165:VAL:HG21	2.01	0.43
1:A:347:ILE:HG12	1:A:392:TYR:CD2	2.54	0.43
1:A:444:SER:OG	1:A:466:PRO:HG2	2.19	0.43
1:A:602:VAL:HA	3:A:1267:HOH:O	2.18	0.43
1:B:638:ASP:HB3	1:B:651:ARG:HB3	2.01	0.43
1:B:861:ARG:HB3	3:B:1236:HOH:O	2.17	0.43
1:C:272:ASP:OD1	1:C:289:LYS:NZ	2.52	0.43
1:C:577:PRO:HG3	1:D:789:GLU:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:770:LYS:O	1:C:777:VAL:HG12	2.18	0.43
1:C:993:GLY:N	1:C:1011:PHE:O	2.51	0.43
1:D:319:ILE:HG23	1:D:677:PRO:HB3	2.00	0.43
1:D:462:ALA:HA	1:D:481:HIS:O	2.19	0.43
1:F:909:ILE:HG12	1:F:956:ILE:CG2	2.48	0.43
1:A:731:LEU:O	1:A:731:LEU:HD22	2.18	0.43
1:B:218:ASN:HB3	1:B:221:ALA:HB3	1.99	0.43
1:B:279:ASN:HA	3:B:1261:HOH:O	2.17	0.43
1:B:442:GLU:OE2	1:B:481:HIS:HD2	2.01	0.43
1:B:765:ILE:HD11	1:B:769:PHE:HZ	1.84	0.43
1:C:648:VAL:O	1:C:659:THR:HA	2.18	0.43
1:C:684:GLU:HG3	1:C:685:GLU:N	2.32	0.43
1:C:994:ILE:HG22	1:C:1008:GLN:C	2.44	0.43
1:D:568:LEU:HB3	1:D:571:MET:CE	2.42	0.43
1:D:929:MET:HE3	1:D:979:LEU:CD1	2.47	0.43
1:E:87:PHE:HB3	1:E:88:PRO:CD	2.40	0.43
1:E:200:PRO:O	1:E:740:GLY:HA3	2.18	0.43
1:E:618:VAL:CG2	1:E:631:GLU:HG3	2.48	0.43
1:E:648:VAL:O	1:E:659:THR:HA	2.19	0.43
1:F:51:ASP:C	3:F:1222:HOH:O	2.59	0.43
1:F:82:ASN:ND2	1:F:96:ARG:HH21	2.15	0.43
1:F:994:ILE:HG22	1:F:1008:GLN:C	2.44	0.43
1:B:515:LEU:HD23	1:B:539:PRO:HA	2.00	0.43
1:C:53:ILE:HD11	1:C:295:ILE:HD11	2.00	0.43
1:C:236:VAL:HG23	1:C:243:TYR:HB2	2.00	0.43
1:E:228:MET:HE1	1:E:244:PHE:CE1	2.53	0.43
1:E:319:ILE:HG23	1:E:677:PRO:HB3	2.01	0.43
1:E:390:TYR:HD1	1:E:397:ALA:HB2	1.83	0.43
1:E:662:LEU:O	1:E:662:LEU:HD12	2.19	0.43
1:F:82:ASN:HD22	1:F:82:ASN:N	2.12	0.43
1:F:93:ILE:HD12	1:F:111:TYR:HD2	1.82	0.43
1:F:131:ARG:HH12	2:F:1214:DKT:CD6	2.32	0.43
1:F:347:ILE:HG12	1:F:392:TYR:CD2	2.54	0.43
1:F:599:SER:HB2	3:F:1302:HOH:O	2.16	0.43
1:A:164:ARG:HD3	3:A:1264:HOH:O	2.18	0.43
1:A:204:GLY:O	1:A:206:ARG:HG3	2.17	0.43
1:B:568:LEU:HB3	1:B:571:MET:CE	2.44	0.43
1:C:687:LEU:HD23	1:C:722:VAL:HG11	2.00	0.43
1:C:894:GLU:HA	1:C:894:GLU:OE2	2.18	0.43
1:D:546:PRO:CG	1:D:567:ASP:HB3	2.49	0.43
1:E:363:ARG:HD3	1:E:363:ARG:HA	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:424:ASP:CB	3:F:1238:HOH:O	2.67	0.43
1:A:765:ILE:HD13	1:A:765:ILE:N	2.33	0.43
1:C:217:VAL:HG23	1:C:218:ASN:N	2.34	0.43
1:C:297:ASN:O	1:C:301:GLU:N	2.48	0.43
1:C:1027:VAL:C	3:C:1217:HOH:O	2.61	0.43
1:D:562:GLU:C	1:D:564:GLY:H	2.27	0.43
1:E:750:MET:HG2	3:E:1284:HOH:O	2.18	0.43
1:F:293:ILE:HG22	1:F:306:ILE:HD12	1.99	0.43
1:A:131:ARG:HH12	2:A:1214:DKT:CD6	2.32	0.43
1:A:618:VAL:CG2	1:A:631:GLU:HG3	2.49	0.43
1:B:540:PHE:HE1	3:B:1307:HOH:O	2.01	0.43
1:C:792:LYS:NZ	3:D:1252:HOH:O	2.37	0.43
1:C:887:MET:HE3	1:C:921:SER:CB	2.48	0.43
1:D:351:SER:OG	1:D:353:THR:CG2	2.63	0.43
1:D:684:GLU:HG3	1:D:685:GLU:N	2.33	0.43
1:F:53:ILE:HG23	1:F:286:LEU:CD2	2.43	0.43
1:F:605:GLU:HG2	3:F:1235:HOH:O	2.18	0.43
1:A:460:PHE:CE2	1:A:568:LEU:HD11	2.53	0.43
1:B:46:PRO:HD3	1:B:288:SER:HB3	1.99	0.43
1:B:201:HIS:O	1:B:740:GLY:HA2	2.19	0.43
1:C:809:ASP:HB3	1:C:814:THR:HA	2.01	0.43
1:C:898:LEU:O	1:C:899:PHE:C	2.62	0.43
1:C:1010:GLU:HB3	1:C:1011:PHE:CE1	2.53	0.43
1:E:131:ARG:NH1	2:E:1214:DKT:HD62	2.34	0.43
1:E:1010:GLU:HB3	1:E:1011:PHE:CD1	2.54	0.43
1:F:353:THR:HG23	1:F:354:TYR:CD1	2.54	0.43
1:F:714:ILE:HG21	1:F:741:GLU:HB3	1.99	0.43
1:A:981:LYS:HB2	3:A:1254:HOH:O	2.18	0.43
1:B:43:LEU:HD22	1:B:55:PHE:CE1	2.53	0.43
1:B:1008:GLN:HE21	1:B:1008:GLN:HB2	1.65	0.43
1:C:201:HIS:O	1:C:740:GLY:HA2	2.19	0.43
1:C:442:GLU:OE2	1:C:481:HIS:HD2	2.02	0.43
1:D:716:GLU:HB3	3:D:1279:HOH:O	2.18	0.43
1:E:322:PRO:HG3	1:E:673:THR:O	2.18	0.43
1:E:706:VAL:HG12	1:E:710:ILE:HG12	1.99	0.43
1:E:799:GLY:O	1:E:800:ILE:HG23	2.17	0.43
1:F:603:HIS:HD2	1:F:604:GLY:O	2.02	0.43
1:F:1039:ASP:CG	3:F:1267:HOH:O	2.61	0.43
1:A:706:VAL:HG12	1:A:710:ILE:HG12	2.01	0.42
1:A:874:ARG:HH11	1:A:1053:ASP:CG	2.27	0.42
1:B:284:ARG:CD	3:B:1222:HOH:O	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:GLY:O	1:B:473:ASP:HB2	2.19	0.42
1:B:562:GLU:C	1:B:564:GLY:H	2.26	0.42
1:B:976:LYS:NZ	1:B:1017:ASP:HB2	2.34	0.42
1:C:131:ARG:NH1	2:C:1214:DKT:HD62	2.34	0.42
1:C:245:ILE:HD12	3:C:1223:HOH:O	2.18	0.42
1:C:367:VAL:CG1	1:C:375:VAL:HG21	2.48	0.42
1:C:498:SER:CB	3:C:1320:HOH:O	2.67	0.42
1:C:545:ILE:N	1:C:545:ILE:HD12	2.34	0.42
1:D:138:ALA:HB1	1:D:183:ILE:HG22	2.00	0.42
1:D:141:ASP:OD2	1:D:141:ASP:C	2.62	0.42
1:D:369:ARG:HH21	1:D:369:ARG:HG3	1.83	0.42
1:D:562:GLU:HA	3:D:1291:HOH:O	2.19	0.42
1:D:569:ASN:O	1:D:570:ASP:C	2.61	0.42
1:D:776:TYR:CE1	1:D:821:ILE:HB	2.53	0.42
1:E:88:PRO:HG2	1:E:89:ASP:H	1.83	0.42
1:E:1014:TRP:CD1	1:E:1019:GLY:HA2	2.53	0.42
1:A:403:ASN:ND2	1:A:403:ASN:C	2.76	0.42
1:A:684:GLU:HG3	1:A:685:GLU:N	2.33	0.42
1:C:234:SER:O	1:C:278:LEU:HB2	2.19	0.42
1:C:362:LEU:HD13	1:C:688:GLN:HG3	2.01	0.42
1:C:467:LEU:C	1:C:467:LEU:HD12	2.44	0.42
1:C:823:ARG:HD2	1:F:317:ARG:CD	2.42	0.42
1:C:909:ILE:HG12	1:C:956:ILE:CG2	2.49	0.42
1:D:96:ARG:HH21	1:D:96:ARG:HG2	1.84	0.42
1:D:687:LEU:HD23	1:D:722:VAL:HG11	2.00	0.42
1:E:369:ARG:HH21	1:E:369:ARG:HG3	1.82	0.42
1:E:578:ILE:O	1:E:580:VAL:N	2.50	0.42
1:E:639:LEU:HD23	1:E:640:ARG:N	2.34	0.42
1:F:43:LEU:HD22	1:F:55:PHE:CE1	2.54	0.42
1:F:882:ILE:HG22	1:F:883:HIS:N	2.34	0.42
1:A:53:ILE:HD11	1:A:295:ILE:HD11	2.01	0.42
1:B:82:ASN:ND2	1:B:96:ARG:HH21	2.16	0.42
1:B:618:VAL:CG2	1:B:631:GLU:HG3	2.49	0.42
1:C:46:PRO:HD3	1:C:288:SER:HB3	2.01	0.42
1:C:890:MET:O	1:C:894:GLU:HG2	2.19	0.42
1:D:228:MET:HE1	1:D:244:PHE:CE1	2.55	0.42
1:D:285:ILE:HD12	1:D:296:PHE:CD2	2.54	0.42
1:D:887:MET:HB2	1:D:917:GLY:C	2.44	0.42
1:E:59:ASP:OD2	1:E:59:ASP:N	2.52	0.42
1:E:64:HIS:HB2	1:E:71:THR:HG23	2.02	0.42
1:E:633:LYS:HB2	1:E:633:LYS:HE2	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:351:SER:CB	1:F:353:THR:HG22	2.49	0.42
1:A:228:MET:HE1	1:A:244:PHE:CE1	2.54	0.42
1:B:162:LEU:HD21	1:B:180:ALA:HB3	2.01	0.42
1:B:390:TYR:HD1	1:B:397:ALA:HB2	1.85	0.42
1:B:546:PRO:CG	1:B:567:ASP:HB3	2.50	0.42
1:B:744:THR:HG22	1:B:745:SER:H	1.82	0.42
1:C:120:ARG:C	1:C:121:ILE:HD12	2.43	0.42
1:D:936:ASP:HB3	1:D:944:SER:HB3	2.01	0.42
1:E:43:LEU:HD22	1:E:55:PHE:CE1	2.54	0.42
1:E:351:SER:CB	1:E:353:THR:HG22	2.49	0.42
1:E:789:GLU:HG3	1:F:577:PRO:HG3	2.01	0.42
1:E:791:GLU:CD	1:E:861:ARG:HE	2.27	0.42
1:F:350:VAL:HG23	1:F:351:SER:N	2.34	0.42
1:A:218:ASN:HB3	1:A:221:ALA:HB3	2.00	0.42
1:A:285:ILE:HD12	1:A:296:PHE:HD2	1.84	0.42
1:A:515:LEU:HD23	1:A:539:PRO:HA	2.01	0.42
1:B:46:PRO:HB2	1:B:286:LEU:CD2	2.50	0.42
1:B:53:ILE:HD11	1:B:295:ILE:HD11	2.02	0.42
1:B:91:ARG:CZ	3:B:1273:HOH:O	2.67	0.42
1:B:1031:VAL:HG12	1:B:1033:ILE:HD12	2.01	0.42
1:C:546:PRO:CG	1:C:567:ASP:HB3	2.50	0.42
1:D:506:ASP:HB2	3:D:1246:HOH:O	2.19	0.42
1:E:131:ARG:HH12	2:E:1214:DKT:HD61	1.83	0.42
1:E:715:TYR:CZ	1:E:719:ARG:HD2	2.55	0.42
1:F:45:ASN:HB3	1:F:277:HIS:CE1	2.54	0.42
1:F:91:ARG:NH1	1:F:114:GLU:HB2	2.35	0.42
1:F:533:PHE:HB3	1:F:536:VAL:HG11	2.01	0.42
1:F:887:MET:HB2	1:F:917:GLY:C	2.44	0.42
1:F:887:MET:HE3	1:F:921:SER:CB	2.49	0.42
1:A:735:ILE:HG22	1:A:739:GLN:HE21	1.84	0.42
1:A:929:MET:HE3	1:A:979:LEU:CD1	2.49	0.42
1:B:82:ASN:HD22	1:B:82:ASN:N	2.14	0.42
1:C:904:SER:CB	1:D:473:ASP:HA	2.49	0.42
1:D:91:ARG:NH1	1:D:114:GLU:HB2	2.34	0.42
1:D:201:HIS:O	1:D:740:GLY:HA2	2.18	0.42
1:E:569:ASN:O	1:E:570:ASP:C	2.62	0.42
1:E:644:ASP:OD2	1:E:646:LYS:HB2	2.20	0.42
1:F:746:HIS:HB2	3:F:1257:HOH:O	2.18	0.42
1:A:184:LEU:HD13	1:A:237:ILE:HG13	2.02	0.42
1:A:882:ILE:HG22	1:A:883:HIS:N	2.34	0.42
1:B:353:THR:HG23	1:B:354:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:746:HIS:HA	1:B:748:TYR:CE2	2.53	0.42
1:C:314:PRO:HA	1:F:118:ILE:HG22	2.00	0.42
1:C:387:LEU:HD22	1:C:388:GLY:H	1.85	0.42
1:C:515:LEU:HD23	1:C:539:PRO:HA	2.01	0.42
1:C:535:VAL:HG12	1:C:583:GLY:HA2	2.01	0.42
1:C:868:ARG:HH12	1:D:497:ASN:HD22	1.67	0.42
1:D:130:GLY:N	3:D:1286:HOH:O	2.52	0.42
1:D:578:ILE:O	1:D:580:VAL:N	2.51	0.42
1:D:890:MET:O	1:D:894:GLU:HG2	2.19	0.42
1:D:898:LEU:O	1:D:899:PHE:C	2.61	0.42
1:E:809:ASP:HB3	1:E:814:THR:HA	2.02	0.42
1:E:840:LYS:N	3:E:1295:HOH:O	2.52	0.42
1:E:871:VAL:HG22	1:E:1052:ILE:CD1	2.44	0.42
1:E:904:SER:CB	1:F:473:ASP:HA	2.50	0.42
1:F:131:ARG:NH1	2:F:1214:DKT:HD62	2.35	0.42
1:F:579:ASN:HB2	3:F:1285:HOH:O	2.20	0.42
1:A:335:ASP:HA	3:A:1262:HOH:O	2.19	0.42
1:A:766:ALA:HB3	1:A:793:SER:CA	2.48	0.42
1:B:59:ASP:OD2	1:B:59:ASP:N	2.50	0.42
1:B:367:VAL:CG1	1:B:375:VAL:HG21	2.50	0.42
1:B:423:ASN:C	1:B:423:ASN:HD22	2.26	0.42
1:C:662:LEU:HD12	1:C:662:LEU:O	2.19	0.42
1:F:993:GLY:N	1:F:1011:PHE:O	2.52	0.42
1:A:162:LEU:HD21	1:A:180:ALA:HB3	2.01	0.42
1:A:530:ASN:HD22	1:A:531:PHE:N	2.10	0.42
1:A:638:ASP:HB3	1:A:651:ARG:HB3	2.01	0.42
1:B:351:SER:CB	1:B:353:THR:HG22	2.50	0.42
1:B:538:LYS:HB3	3:B:1307:HOH:O	2.19	0.42
1:C:293:ILE:HG22	1:C:306:ILE:HD12	2.01	0.42
1:D:526:ARG:NH1	3:D:1288:HOH:O	2.52	0.42
1:E:53:ILE:HD11	1:E:295:ILE:HD11	2.02	0.42
1:F:201:HIS:O	1:F:740:GLY:HA2	2.20	0.42
1:F:217:VAL:HG23	1:F:218:ASN:N	2.35	0.42
1:F:648:VAL:O	1:F:659:THR:HA	2.19	0.42
1:A:120:ARG:C	1:A:121:ILE:HD12	2.45	0.42
1:B:421:VAL:CB	1:B:429:MET:HE3	2.43	0.42
1:B:624:VAL:HG23	1:B:625:LYS:N	2.35	0.42
1:C:351:SER:OG	1:C:353:THR:CG2	2.63	0.42
1:C:605:GLU:HG2	1:D:524:PRO:HD3	2.01	0.42
1:C:799:GLY:O	1:C:800:ILE:HG23	2.20	0.42
1:D:46:PRO:HD3	1:D:288:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:715:TYR:CZ	1:D:719:ARG:HD2	2.55	0.42
1:D:882:ILE:HD11	1:D:899:PHE:HA	2.02	0.42
1:D:929:MET:HB3	3:D:1219:HOH:O	2.19	0.42
1:F:300:THR:HG22	1:F:302:LYS:HB2	2.01	0.42
1:F:414:ARG:NH1	1:F:644:ASP:HA	2.35	0.42
1:F:618:VAL:CG2	1:F:631:GLU:HG3	2.50	0.42
1:A:521:ASP:CG	1:B:604:GLY:HA3	2.45	0.41
1:A:770:LYS:O	1:A:777:VAL:HG12	2.20	0.41
1:B:184:LEU:HB2	1:B:191:VAL:HB	2.02	0.41
1:C:524:PRO:HD3	1:D:605:GLU:HG2	2.01	0.41
1:C:532:SER:OG	1:C:534:GLU:OE1	2.38	0.41
1:C:744:THR:HG22	1:C:745:SER:H	1.82	0.41
1:D:532:SER:OG	1:D:534:GLU:OE1	2.38	0.41
1:D:710:ILE:HD13	1:D:713:ARG:NH2	2.35	0.41
1:E:887:MET:HE3	1:E:921:SER:CB	2.50	0.41
1:F:452:PHE:CB	1:F:463:TYR:HB3	2.51	0.41
1:F:546:PRO:CG	1:F:567:ASP:HB3	2.49	0.41
1:F:809:ASP:HB3	1:F:814:THR:HA	2.02	0.41
1:A:363:ARG:HD3	1:A:363:ARG:HA	1.77	0.41
1:A:546:PRO:CG	1:A:567:ASP:HB3	2.50	0.41
1:B:217:VAL:HG23	1:B:218:ASN:N	2.35	0.41
1:C:386:PHE:N	1:C:386:PHE:CD1	2.88	0.41
1:C:633:LYS:HE2	1:C:633:LYS:HB2	1.88	0.41
1:C:771:LEU:HD13	3:C:1234:HOH:O	2.19	0.41
1:C:874:ARG:HH11	1:C:1053:ASP:CG	2.28	0.41
1:D:64:HIS:HB2	1:D:71:THR:HG23	2.01	0.41
1:D:109:TYR:CE2	1:D:120:ARG:HB2	2.55	0.41
1:D:387:LEU:HD22	1:D:388:GLY:H	1.84	0.41
1:D:421:VAL:CB	1:D:429:MET:HE3	2.46	0.41
1:D:573:LYS:HA	3:D:1252:HOH:O	2.21	0.41
1:D:799:GLY:O	1:D:800:ILE:HG23	2.19	0.41
1:E:155:PRO:HG2	1:E:156:PHE:CD1	2.54	0.41
1:E:605:GLU:HG3	1:F:524:PRO:HD3	2.02	0.41
1:E:936:ASP:HB3	1:E:944:SER:HB3	2.02	0.41
1:F:59:ASP:OD2	1:F:59:ASP:N	2.53	0.41
1:F:155:PRO:HG2	1:F:156:PHE:CD1	2.55	0.41
1:F:746:HIS:HA	1:F:748:TYR:CE2	2.55	0.41
1:F:764:ARG:HG2	1:F:764:ARG:HH21	1.85	0.41
1:A:1010:GLU:HB3	1:A:1011:PHE:CD1	2.55	0.41
1:B:155:PRO:HG2	1:B:156:PHE:CD1	2.56	0.41
1:B:285:ILE:HD12	1:B:296:PHE:CD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:809:ASP:HB3	1:B:814:THR:HA	2.02	0.41
1:B:936:ASP:HB3	1:B:944:SER:HB3	2.00	0.41
1:C:82:ASN:HD21	1:C:96:ARG:HH21	1.67	0.41
1:C:363:ARG:HD3	1:C:363:ARG:HA	1.79	0.41
1:C:568:LEU:HB3	1:C:571:MET:CE	2.46	0.41
1:C:1008:GLN:HE21	1:C:1008:GLN:HB2	1.68	0.41
1:D:44:LEU:HD13	1:D:733:ASN:ND2	2.35	0.41
1:D:874:ARG:HH11	1:D:1053:ASP:CG	2.28	0.41
1:F:662:LEU:HD12	1:F:662:LEU:O	2.21	0.41
1:F:872:HIS:HE1	1:F:902:GLU:OE1	2.03	0.41
1:A:91:ARG:NH1	1:A:114:GLU:HB2	2.36	0.41
1:A:285:ILE:HD12	1:A:296:PHE:CD2	2.56	0.41
1:A:351:SER:OG	1:A:353:THR:CG2	2.65	0.41
1:A:578:ILE:O	1:A:580:VAL:N	2.54	0.41
1:B:194:ARG:HD2	3:B:1279:HOH:O	2.20	0.41
1:C:285:ILE:HD12	1:C:296:PHE:CD2	2.56	0.41
1:C:530:ASN:HD22	1:C:531:PHE:N	2.13	0.41
1:D:88:PRO:HG2	1:D:89:ASP:H	1.84	0.41
1:D:272:ASP:OD1	1:D:289:LYS:NZ	2.53	0.41
1:E:54:ILE:HG23	1:E:86:PHE:CZ	2.56	0.41
1:E:146:LEU:HD23	1:E:165:VAL:HG21	2.02	0.41
1:E:295:ILE:HG13	1:E:306:ILE:HD11	2.03	0.41
1:E:891:GLY:C	3:E:1244:HOH:O	2.63	0.41
1:F:270:PHE:CD2	1:F:289:LYS:HE2	2.55	0.41
1:A:131:ARG:HH12	2:A:1214:DKT:HD61	1.85	0.41
1:A:367:VAL:CG1	1:A:375:VAL:HG21	2.51	0.41
1:A:462:ALA:HA	1:A:481:HIS:O	2.20	0.41
1:A:522:PRO:CG	1:B:889:MET:SD	3.07	0.41
1:A:715:TYR:CZ	1:A:719:ARG:HD2	2.55	0.41
1:B:731:LEU:HD13	1:B:735:ILE:HD12	2.03	0.41
1:B:753:THR:HB	3:B:1319:HOH:O	2.21	0.41
1:C:45:ASN:HB3	1:C:277:HIS:CE1	2.55	0.41
1:C:124:PHE:HB3	1:C:152:ALA:HB1	2.01	0.41
1:C:175:LEU:O	1:C:177:LEU:HG	2.20	0.41
1:C:706:VAL:HG12	1:C:710:ILE:HG12	2.02	0.41
1:F:936:ASP:HB3	1:F:944:SER:HB3	2.01	0.41
1:A:414:ARG:NH1	1:A:644:ASP:HA	2.35	0.41
1:B:131:ARG:HH12	2:B:1214:DKT:HD61	1.85	0.41
1:B:565:GLU:HG2	1:B:566:TYR:N	2.35	0.41
1:B:706:VAL:HG12	1:B:710:ILE:HG12	2.02	0.41
1:B:929:MET:HE3	1:B:979:LEU:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:PRO:HG3	1:C:673:THR:O	2.20	0.41
1:D:467:LEU:HD21	1:D:496:GLU:HB3	2.02	0.41
1:E:470:GLY:O	1:E:473:ASP:HB2	2.20	0.41
1:E:904:SER:OG	1:F:473:ASP:HA	2.20	0.41
1:F:120:ARG:C	1:F:121:ILE:HD12	2.46	0.41
1:F:537:SER:HB3	1:F:583:GLY:O	2.21	0.41
1:F:929:MET:HE3	1:F:979:LEU:CD1	2.48	0.41
1:A:693:ALA:HB2	1:A:1006:LEU:HD11	2.03	0.41
1:B:467:LEU:HD21	1:B:496:GLU:HB3	2.03	0.41
1:B:569:ASN:O	1:B:570:ASP:C	2.62	0.41
1:C:425:ARG:O	1:C:426:PHE:HB2	2.20	0.41
1:C:681:SER:OG	1:C:684:GLU:HG2	2.21	0.41
1:E:45:ASN:N	1:E:45:ASN:ND2	2.66	0.41
1:E:497:ASN:ND2	1:F:868:ARG:HH12	2.19	0.41
1:E:694:TRP:HA	1:E:738:MET:CE	2.51	0.41
1:E:887:MET:C	1:E:920:VAL:HG22	2.46	0.41
1:F:65:ASP:CA	3:F:1222:HOH:O	2.65	0.41
1:A:442:GLU:OE2	1:A:481:HIS:HD2	2.04	0.41
1:B:54:ILE:HG23	1:B:86:PHE:CZ	2.55	0.41
1:B:253:GLN:NE2	1:B:253:GLN:HA	2.35	0.41
1:B:840:LYS:N	3:B:1294:HOH:O	2.54	0.41
1:B:1010:GLU:HB3	1:B:1011:PHE:CD1	2.56	0.41
1:C:777:VAL:HG22	1:C:778:VAL:N	2.35	0.41
1:D:253:GLN:NE2	1:D:253:GLN:HA	2.36	0.41
1:D:764:ARG:HH21	1:D:764:ARG:HG2	1.85	0.41
1:E:346:PHE:C	1:E:347:ILE:HD12	2.45	0.41
1:F:46:PRO:HB2	1:F:286:LEU:CD2	2.51	0.41
1:F:369:ARG:HH21	1:F:369:ARG:HG3	1.85	0.41
1:F:729:TYR:O	1:F:732:SER:HB3	2.21	0.41
1:F:1014:TRP:NE1	1:F:1019:GLY:HA2	2.36	0.41
1:A:43:LEU:HD22	1:A:55:PHE:CE1	2.55	0.41
1:A:131:ARG:NH1	2:A:1214:DKT:HD62	2.35	0.41
1:A:147:ILE:CD1	3:A:1264:HOH:O	2.69	0.41
1:A:256:SER:OG	1:A:267:HIS:CE1	2.70	0.41
1:A:1031:VAL:HG12	1:A:1033:ILE:HD12	2.02	0.41
1:B:91:ARG:NH2	3:B:1273:HOH:O	2.53	0.41
1:B:92:LYS:C	1:B:93:ILE:HG13	2.46	0.41
1:B:131:ARG:NH1	2:B:1214:DKT:HD62	2.36	0.41
1:B:236:VAL:HG23	1:B:243:TYR:HB2	2.01	0.41
1:B:287:PHE:CZ	1:B:294:TYR:HB2	2.56	0.41
1:B:369:ARG:HG3	1:B:369:ARG:HH21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:HIS:HD2	1:B:604:GLY:O	2.04	0.41
1:B:994:ILE:HG22	1:B:1008:GLN:C	2.46	0.41
1:C:93:ILE:HD12	1:C:111:TYR:HD2	1.85	0.41
1:C:448:MET:HB2	3:C:1277:HOH:O	2.20	0.41
1:C:715:TYR:CZ	1:C:719:ARG:HD2	2.56	0.41
1:C:1031:VAL:HG11	1:C:1050:TYR:CZ	2.56	0.41
1:D:45:ASN:HB3	1:D:277:HIS:CE1	2.56	0.41
1:D:349:ASP:O	1:D:350:VAL:C	2.64	0.41
1:D:403:ASN:ND2	1:D:403:ASN:C	2.75	0.41
1:D:425:ARG:O	1:D:426:PHE:HB2	2.21	0.41
1:D:644:ASP:OD2	1:D:646:LYS:HB2	2.20	0.41
1:D:1010:GLU:HB3	1:D:1011:PHE:CD1	2.56	0.41
1:E:134:PHE:CB	3:E:1286:HOH:O	2.54	0.41
1:E:525:ASP:CG	1:F:533:PHE:H	2.28	0.41
1:E:562:GLU:C	1:E:564:GLY:H	2.28	0.41
1:F:203:LYS:HE3	1:F:741:GLU:OE1	2.21	0.41
1:F:222:PHE:H	1:F:1038:HIS:HD2	1.69	0.41
1:F:236:VAL:HG23	1:F:243:TYR:HB2	2.03	0.41
1:F:297:ASN:O	1:F:301:GLU:N	2.46	0.41
1:F:423:ASN:C	1:F:423:ASN:HD22	2.28	0.41
1:F:644:ASP:OD2	1:F:646:LYS:HB2	2.21	0.41
1:F:1010:GLU:HB3	1:F:1011:PHE:CD1	2.55	0.41
1:A:217:VAL:HG23	1:A:218:ASN:N	2.36	0.41
1:A:313:SER:O	1:D:117:GLU:HA	2.21	0.41
1:A:423:ASN:C	1:A:423:ASN:HD22	2.29	0.41
1:A:764:ARG:HG2	1:A:764:ARG:HH21	1.86	0.41
1:B:764:ARG:HG2	1:B:764:ARG:HH21	1.86	0.41
1:B:993:GLY:N	1:B:1011:PHE:O	2.54	0.41
1:C:131:ARG:HH12	2:C:1214:DKT:HD61	1.86	0.41
1:C:353:THR:HG23	1:C:354:TYR:CD1	2.55	0.41
1:C:524:PRO:HD3	1:D:605:GLU:HG3	2.02	0.41
1:C:976:LYS:NZ	1:C:1017:ASP:HB2	2.36	0.41
1:D:125:SER:CB	1:D:762:SER:HB2	2.50	0.41
1:D:253:GLN:HA	1:D:253:GLN:HE21	1.86	0.41
1:E:317:ARG:CZ	3:E:1226:HOH:O	2.69	0.41
1:E:522:PRO:HG2	1:F:889:MET:SD	2.61	0.41
1:E:728:ARG:HG3	1:E:754:PHE:CE1	2.56	0.41
1:E:731:LEU:HD13	1:E:735:ILE:HD12	2.01	0.41
1:F:578:ILE:O	1:F:580:VAL:N	2.54	0.41
1:A:489:LYS:HE2	1:A:491:PHE:HZ	1.85	0.40
1:A:993:GLY:N	1:A:1011:PHE:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:ARG:NH2	3:B:1281:HOH:O	2.37	0.40
1:B:387:LEU:HD22	1:B:388:GLY:H	1.86	0.40
1:B:532:SER:OG	1:B:534:GLU:OE1	2.39	0.40
1:B:770:LYS:O	1:B:777:VAL:HG12	2.21	0.40
1:C:369:ARG:HG3	1:C:369:ARG:HH21	1.86	0.40
1:C:906:GLN:O	1:C:953:GLY:HA3	2.22	0.40
1:C:1010:GLU:HB3	1:C:1011:PHE:CD1	2.56	0.40
1:E:203:LYS:HE3	1:E:741:GLU:OE1	2.20	0.40
1:F:387:LEU:HD22	1:F:388:GLY:H	1.86	0.40
1:F:499:HIS:CD2	3:F:1263:HOH:O	2.71	0.40
1:F:776:TYR:CE1	1:F:821:ILE:HB	2.56	0.40
1:F:1036:ALA:C	3:F:1267:HOH:O	2.63	0.40
1:B:53:ILE:HG23	1:B:286:LEU:CD2	2.45	0.40
1:B:184:LEU:HD13	1:B:237:ILE:HG13	2.02	0.40
1:B:272:ASP:OD1	1:B:289:LYS:NZ	2.54	0.40
1:B:715:TYR:CZ	1:B:719:ARG:HD2	2.56	0.40
1:C:1014:TRP:NE1	1:C:1019:GLY:HA2	2.36	0.40
1:D:884:ILE:HG22	1:D:886:ASP:O	2.21	0.40
1:E:201:HIS:O	1:E:740:GLY:HA2	2.22	0.40
1:E:1000:LEU:HB2	1:E:1004:THR:HB	2.04	0.40
1:A:46:PRO:HD3	1:A:288:SER:HB3	2.02	0.40
1:A:147:ILE:HD11	3:A:1264:HOH:O	2.21	0.40
1:A:904:SER:OG	1:B:473:ASP:HA	2.22	0.40
1:B:243:TYR:CD2	1:B:256:SER:HB3	2.55	0.40
1:B:965:SER:C	1:B:967:GLY:N	2.79	0.40
1:C:368:ARG:CZ	3:C:1251:HOH:O	2.69	0.40
1:C:393:ARG:HH12	1:E:557:ARG:HG3	1.87	0.40
1:C:423:ASN:C	1:C:423:ASN:HD22	2.28	0.40
1:C:660:PHE:HB3	1:C:668:GLU:CB	2.50	0.40
1:D:287:PHE:CZ	1:D:294:TYR:HB2	2.57	0.40
1:E:46:PRO:HD3	1:E:288:SER:HB3	2.03	0.40
1:E:710:ILE:HD13	1:E:713:ARG:NH2	2.36	0.40
1:E:776:TYR:CE1	1:E:821:ILE:HB	2.56	0.40
1:F:184:LEU:HD13	1:F:237:ILE:HG13	2.03	0.40
1:F:976:LYS:NZ	1:F:1017:ASP:HB2	2.36	0.40
1:A:317:ARG:HB3	3:A:1294:HOH:O	2.21	0.40
1:A:746:HIS:HA	1:A:748:TYR:CE2	2.56	0.40
1:A:886:ASP:OD2	1:A:886:ASP:C	2.65	0.40
1:B:913:ARG:O	1:B:914:PHE:HB2	2.20	0.40
1:C:287:PHE:CZ	1:C:294:TYR:HB2	2.57	0.40
1:C:912:VAL:HG11	1:C:970:PHE:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:977:LEU:HB2	1:C:979:LEU:HD13	2.03	0.40
1:E:467:LEU:HD21	1:E:496:GLU:HB3	2.03	0.40
1:E:532:SER:OG	1:E:534:GLU:OE1	2.39	0.40
1:E:684:GLU:HG3	1:E:685:GLU:N	2.35	0.40
1:E:768:ASP:HB2	1:E:780:LYS:HB3	2.04	0.40
1:F:380:GLY:C	3:F:1251:HOH:O	2.64	0.40
1:F:526:ARG:NH2	3:F:1225:HOH:O	2.53	0.40
1:F:886:ASP:OD2	1:F:886:ASP:C	2.65	0.40
1:F:977:LEU:HB2	1:F:979:LEU:HD13	2.03	0.40
1:A:164:ARG:CG	3:A:1264:HOH:O	2.65	0.40
1:A:300:THR:HG22	1:A:302:LYS:HB2	2.04	0.40
1:A:312:GLU:HG2	1:A:314:PRO:HD3	2.02	0.40
1:A:532:SER:OG	1:A:534:GLU:OE1	2.39	0.40
1:A:701:TYR:O	1:B:939:ARG:HD3	2.22	0.40
1:B:256:SER:OG	1:B:267:HIS:CE1	2.72	0.40
1:B:414:ARG:NH1	1:B:644:ASP:HA	2.37	0.40
1:B:703:ASN:C	1:B:703:ASN:ND2	2.79	0.40
1:C:59:ASP:OD2	1:C:59:ASP:N	2.54	0.40
1:C:91:ARG:NH1	1:C:114:GLU:HB2	2.36	0.40
1:C:537:SER:HB3	1:C:583:GLY:O	2.22	0.40
1:C:562:GLU:C	1:C:564:GLY:N	2.79	0.40
1:D:365:ARG:NH2	3:D:1341:HOH:O	2.38	0.40
1:D:648:VAL:O	1:D:659:THR:HA	2.21	0.40
1:D:1000:LEU:HB2	1:D:1004:THR:HB	2.03	0.40
1:E:125:SER:CB	1:E:762:SER:HB2	2.51	0.40
1:E:236:VAL:HG23	1:E:243:TYR:HB2	2.03	0.40
1:E:407:VAL:O	1:E:998:ARG:NH1	2.55	0.40
1:E:882:ILE:HD11	1:E:899:PHE:HA	2.03	0.40
1:E:887:MET:HB2	1:E:917:GLY:C	2.47	0.40
1:F:218:ASN:HB3	1:F:221:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1021/1071 (95%)	950 (93%)	66 (6%)	5 (0%)	24	48
1	B	1021/1071 (95%)	948 (93%)	68 (7%)	5 (0%)	24	48
1	C	1021/1071 (95%)	947 (93%)	69 (7%)	5 (0%)	24	48
1	D	1021/1071 (95%)	955 (94%)	61 (6%)	5 (0%)	24	48
1	E	1021/1071 (95%)	951 (93%)	65 (6%)	5 (0%)	24	48
1	F	1021/1071 (95%)	946 (93%)	69 (7%)	6 (1%)	21	44
All	All	6126/6426 (95%)	5697 (93%)	398 (6%)	31 (0%)	24	48

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	579	ASN
1	B	579	ASN
1	C	579	ASN
1	D	579	ASN
1	E	579	ASN
1	F	579	ASN
1	A	562	GLU
1	B	562	GLU
1	C	562	GLU
1	D	562	GLU
1	E	562	GLU
1	F	562	GLU
1	A	220	GLY
1	A	259	LEU
1	B	220	GLY
1	B	259	LEU
1	C	220	GLY
1	D	220	GLY
1	E	220	GLY
1	F	220	GLY
1	C	259	LEU
1	C	919	PHE
1	D	259	LEU
1	D	919	PHE
1	E	259	LEU
1	E	919	PHE
1	F	259	LEU

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Mol	Chain	Res	Type
1	F	919	PHE
1	B	919	PHE
1	A	919	PHE
1	F	1009	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	883/928 (95%)	847 (96%)	36 (4%)	27	56
1	B	882/928 (95%)	845 (96%)	37 (4%)	26	55
1	C	882/928 (95%)	843 (96%)	39 (4%)	25	53
1	D	882/928 (95%)	843 (96%)	39 (4%)	25	53
1	E	883/928 (95%)	847 (96%)	36 (4%)	27	56
1	F	882/928 (95%)	845 (96%)	37 (4%)	26	55
All	All	5294/5568 (95%)	5070 (96%)	224 (4%)	26	55

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	PRO
1	A	59	ASP
1	A	61	LEU
1	A	75	VAL
1	A	82	ASN
1	A	104	ASN
1	A	128	SER
1	A	209	THR
1	A	260	ASP
1	A	279	ASN
1	A	293	ILE
1	A	311	LEU
1	A	351	SER
1	A	353	THR

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Mol	Chain	Res	Type
1	A	368	ARG
1	A	369	ARG
1	A	423	ASN
1	A	473	ASP
1	A	496	GLU
1	A	562	GLU
1	A	578	ILE
1	A	580	VAL
1	A	588	ILE
1	A	593	SER
1	A	681	SER
1	A	731	LEU
1	A	738	MET
1	A	764	ARG
1	A	765	ILE
1	A	772	ASP
1	A	847	LEU
1	A	853	ASP
1	A	892	LEU
1	A	929	MET
1	A	1008	GLN
1	A	1033	ILE
1	B	46	PRO
1	B	59	ASP
1	B	61	LEU
1	B	71	THR
1	B	75	VAL
1	B	82	ASN
1	B	104	ASN
1	B	128	SER
1	B	209	THR
1	B	260	ASP
1	B	279	ASN
1	B	293	ILE
1	B	311	LEU
1	B	353	THR
1	B	368	ARG
1	B	369	ARG
1	B	423	ASN
1	B	434	GLU
1	B	473	ASP
1	B	496	GLU

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Mol	Chain	Res	Type
1	B	562	GLU
1	B	578	ILE
1	B	580	VAL
1	B	588	ILE
1	B	593	SER
1	B	681	SER
1	B	731	LEU
1	B	738	MET
1	B	764	ARG
1	B	765	ILE
1	B	772	ASP
1	B	847	LEU
1	B	853	ASP
1	B	892	LEU
1	B	929	MET
1	B	1008	GLN
1	B	1015	PHE
1	C	59	ASP
1	C	61	LEU
1	C	71	THR
1	C	75	VAL
1	C	82	ASN
1	C	97	VAL
1	C	104	ASN
1	C	128	SER
1	C	209	THR
1	C	260	ASP
1	C	279	ASN
1	C	293	ILE
1	C	311	LEU
1	C	353	THR
1	C	368	ARG
1	C	369	ARG
1	C	403	ASN
1	C	423	ASN
1	C	429	MET
1	C	434	GLU
1	C	473	ASP
1	C	496	GLU
1	C	562	GLU
1	C	578	ILE
1	C	580	VAL

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Mol	Chain	Res	Type
1	C	588	ILE
1	C	593	SER
1	C	681	SER
1	C	731	LEU
1	C	738	MET
1	C	764	ARG
1	C	765	ILE
1	C	772	ASP
1	C	809	ASP
1	C	847	LEU
1	C	853	ASP
1	C	892	LEU
1	C	929	MET
1	C	1008	GLN
1	D	59	ASP
1	D	61	LEU
1	D	71	THR
1	D	75	VAL
1	D	82	ASN
1	D	97	VAL
1	D	104	ASN
1	D	128	SER
1	D	209	THR
1	D	260	ASP
1	D	279	ASN
1	D	293	ILE
1	D	311	LEU
1	D	351	SER
1	D	353	THR
1	D	368	ARG
1	D	369	ARG
1	D	423	ASN
1	D	434	GLU
1	D	473	ASP
1	D	496	GLU
1	D	562	GLU
1	D	578	ILE
1	D	580	VAL
1	D	588	ILE
1	D	593	SER
1	D	681	SER
1	D	731	LEU

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Mol	Chain	Res	Type
1	D	738	MET
1	D	764	ARG
1	D	765	ILE
1	D	772	ASP
1	D	809	ASP
1	D	847	LEU
1	D	853	ASP
1	D	892	LEU
1	D	929	MET
1	D	1008	GLN
1	D	1015	PHE
1	E	46	PRO
1	E	59	ASP
1	E	61	LEU
1	E	75	VAL
1	E	82	ASN
1	E	97	VAL
1	E	104	ASN
1	E	128	SER
1	E	209	THR
1	E	260	ASP
1	E	279	ASN
1	E	293	ILE
1	E	311	LEU
1	E	353	THR
1	E	368	ARG
1	E	369	ARG
1	E	423	ASN
1	E	473	ASP
1	E	496	GLU
1	E	562	GLU
1	E	578	ILE
1	E	580	VAL
1	E	588	ILE
1	E	593	SER
1	E	681	SER
1	E	731	LEU
1	E	738	MET
1	E	765	ILE
1	E	772	ASP
1	E	809	ASP
1	E	847	LEU

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Mol	Chain	Res	Type
1	E	853	ASP
1	E	892	LEU
1	E	929	MET
1	E	965	SER
1	E	1008	GLN
1	F	46	PRO
1	F	59	ASP
1	F	61	LEU
1	F	71	THR
1	F	75	VAL
1	F	82	ASN
1	F	97	VAL
1	F	104	ASN
1	F	128	SER
1	F	260	ASP
1	F	279	ASN
1	F	293	ILE
1	F	311	LEU
1	F	353	THR
1	F	368	ARG
1	F	369	ARG
1	F	403	ASN
1	F	423	ASN
1	F	434	GLU
1	F	473	ASP
1	F	496	GLU
1	F	562	GLU
1	F	578	ILE
1	F	580	VAL
1	F	588	ILE
1	F	593	SER
1	F	681	SER
1	F	731	LEU
1	F	738	MET
1	F	765	ILE
1	F	772	ASP
1	F	809	ASP
1	F	847	LEU
1	F	853	ASP
1	F	892	LEU
1	F	929	MET
1	F	1008	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (192) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	82	ASN
1	A	104	ASN
1	A	112	ASN
1	A	145	ASN
1	A	253	GLN
1	A	267	HIS
1	A	279	ASN
1	A	297	ASN
1	A	403	ASN
1	A	406	ASN
1	A	415	ASN
1	A	423	ASN
1	A	469	HIS
1	A	481	HIS
1	A	497	ASN
1	A	499	HIS
1	A	511	ASN
1	A	530	ASN
1	A	569	ASN
1	A	603	HIS
1	A	635	ASN
1	A	703	ASN
1	A	733	ASN
1	A	739	GLN
1	A	867	ASN
1	A	872	HIS
1	A	922	GLN
1	A	930	ASN
1	A	949	ASN
1	A	1008	GLN
1	A	1024	ASN
1	A	1047	GLN
1	B	64	HIS
1	B	82	ASN
1	B	104	ASN
1	B	195	ASN
1	B	201	HIS
1	B	253	GLN
1	B	267	HIS
1	B	279	ASN

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Mol	Chain	Res	Type
1	B	297	ASN
1	B	403	ASN
1	B	406	ASN
1	B	415	ASN
1	B	423	ASN
1	B	469	HIS
1	B	481	HIS
1	B	497	ASN
1	B	511	ASN
1	B	530	ASN
1	B	569	ASN
1	B	603	HIS
1	B	635	ASN
1	B	703	ASN
1	B	733	ASN
1	B	739	GLN
1	B	867	ASN
1	B	872	HIS
1	B	922	GLN
1	B	930	ASN
1	B	949	ASN
1	B	1008	GLN
1	B	1024	ASN
1	B	1047	GLN
1	C	64	HIS
1	C	82	ASN
1	C	104	ASN
1	C	112	ASN
1	C	195	ASN
1	C	253	GLN
1	C	267	HIS
1	C	297	ASN
1	C	403	ASN
1	C	406	ASN
1	C	415	ASN
1	C	423	ASN
1	C	469	HIS
1	C	481	HIS
1	C	497	ASN
1	C	499	HIS
1	C	530	ASN
1	C	569	ASN

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Mol	Chain	Res	Type
1	C	603	HIS
1	C	703	ASN
1	C	733	ASN
1	C	739	GLN
1	C	867	ASN
1	C	872	HIS
1	C	922	GLN
1	C	930	ASN
1	C	949	ASN
1	C	1008	GLN
1	C	1024	ASN
1	C	1038	HIS
1	C	1047	GLN
1	D	64	HIS
1	D	82	ASN
1	D	104	ASN
1	D	218	ASN
1	D	253	GLN
1	D	267	HIS
1	D	279	ASN
1	D	297	ASN
1	D	403	ASN
1	D	406	ASN
1	D	415	ASN
1	D	423	ASN
1	D	469	HIS
1	D	481	HIS
1	D	497	ASN
1	D	499	HIS
1	D	530	ASN
1	D	569	ASN
1	D	603	HIS
1	D	635	ASN
1	D	703	ASN
1	D	733	ASN
1	D	739	GLN
1	D	867	ASN
1	D	872	HIS
1	D	922	GLN
1	D	930	ASN
1	D	949	ASN
1	D	1008	GLN

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Mol	Chain	Res	Type
1	D	1024	ASN
1	D	1038	HIS
1	D	1047	GLN
1	E	64	HIS
1	E	82	ASN
1	E	104	ASN
1	E	195	ASN
1	E	253	GLN
1	E	267	HIS
1	E	279	ASN
1	E	297	ASN
1	E	403	ASN
1	E	406	ASN
1	E	415	ASN
1	E	423	ASN
1	E	469	HIS
1	E	481	HIS
1	E	497	ASN
1	E	499	HIS
1	E	511	ASN
1	E	530	ASN
1	E	569	ASN
1	E	603	HIS
1	E	635	ASN
1	E	703	ASN
1	E	733	ASN
1	E	739	GLN
1	E	867	ASN
1	E	872	HIS
1	E	922	GLN
1	E	930	ASN
1	E	949	ASN
1	E	1008	GLN
1	E	1024	ASN
1	E	1047	GLN
1	F	64	HIS
1	F	82	ASN
1	F	104	ASN
1	F	112	ASN
1	F	195	ASN
1	F	201	HIS
1	F	253	GLN

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Mol	Chain	Res	Type
1	F	267	HIS
1	F	279	ASN
1	F	297	ASN
1	F	403	ASN
1	F	406	ASN
1	F	415	ASN
1	F	423	ASN
1	F	469	HIS
1	F	481	HIS
1	F	497	ASN
1	F	499	HIS
1	F	530	ASN
1	F	569	ASN
1	F	603	HIS
1	F	703	ASN
1	F	733	ASN
1	F	739	GLN
1	F	867	ASN
1	F	872	HIS
1	F	922	GLN
1	F	930	ASN
1	F	949	ASN
1	F	1008	GLN
1	F	1024	ASN
1	F	1047	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DKT	B	1214	-	55,57,57	3.85	26 (47%)	66,74,74	5.27	38 (57%)
2	DKT	C	1214	-	55,57,57	3.84	26 (47%)	66,74,74	5.26	38 (57%)
2	DKT	F	1214	-	55,57,57	3.85	26 (47%)	66,74,74	5.27	38 (57%)
2	DKT	D	1214	-	55,57,57	3.85	26 (47%)	66,74,74	5.27	38 (57%)
2	DKT	E	1214	-	55,57,57	3.85	26 (47%)	66,74,74	5.27	38 (57%)
2	DKT	A	1214	-	55,57,57	3.85	26 (47%)	66,74,74	5.27	38 (57%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DKT	B	1214	-	1/1/14/19	27/61/77/77	0/3/3/3
2	DKT	C	1214	-	1/1/14/19	27/61/77/77	0/3/3/3
2	DKT	F	1214	-	1/1/14/19	27/61/77/77	0/3/3/3
2	DKT	D	1214	-	1/1/14/19	27/61/77/77	0/3/3/3
2	DKT	E	1214	-	1/1/14/19	27/61/77/77	0/3/3/3
2	DKT	A	1214	-	1/1/14/19	27/61/77/77	0/3/3/3

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1214	DKT	C4-C5	9.77	1.55	1.38
2	D	1214	DKT	C4-C5	9.77	1.55	1.38
2	A	1214	DKT	C4-C5	9.72	1.55	1.38
2	E	1214	DKT	C4-C5	9.72	1.55	1.38
2	F	1214	DKT	C4-C5	9.70	1.55	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1214	DKT	C4-C5	9.66	1.55	1.38
2	F	1214	DKT	C3-C2	9.62	1.55	1.38
2	D	1214	DKT	C3-C2	9.61	1.55	1.38
2	B	1214	DKT	C3-C2	9.60	1.55	1.38
2	A	1214	DKT	C3-C2	9.59	1.55	1.38
2	E	1214	DKT	C3-C2	9.59	1.55	1.38
2	C	1214	DKT	C3-C2	9.58	1.55	1.38
2	F	1214	DKT	C2-CC3	8.34	1.55	1.38
2	C	1214	DKT	C2-CC3	8.33	1.55	1.38
2	B	1214	DKT	C2-CC3	8.32	1.55	1.38
2	E	1214	DKT	C2-CC3	8.30	1.55	1.38
2	A	1214	DKT	C2-CC3	8.29	1.55	1.38
2	D	1214	DKT	C2-CC3	8.29	1.55	1.38
2	C	1214	DKT	C5-CC3	8.18	1.55	1.38
2	F	1214	DKT	C5-CC3	8.17	1.55	1.38
2	E	1214	DKT	C5-CC3	8.15	1.55	1.38
2	B	1214	DKT	C5-CC3	8.15	1.55	1.38
2	A	1214	DKT	C5-CC3	8.13	1.55	1.38
2	D	1214	DKT	C5-CC3	8.11	1.54	1.38
2	D	1214	DKT	C1-C3	7.78	1.55	1.38
2	E	1214	DKT	C1-C3	7.77	1.55	1.38
2	C	1214	DKT	C1-C3	7.76	1.55	1.38
2	F	1214	DKT	C1-C3	7.76	1.55	1.38
2	B	1214	DKT	C1-C3	7.75	1.55	1.38
2	A	1214	DKT	C1-C3	7.73	1.55	1.38
2	C	1214	DKT	C4-C1	7.68	1.55	1.38
2	B	1214	DKT	C4-C1	7.68	1.55	1.38
2	E	1214	DKT	C4-C1	7.66	1.55	1.38
2	D	1214	DKT	C4-C1	7.66	1.55	1.38
2	A	1214	DKT	C4-C1	7.65	1.55	1.38
2	F	1214	DKT	C4-C1	7.65	1.55	1.38
2	A	1214	DKT	CA1-N	-6.42	1.32	1.45
2	B	1214	DKT	CA1-N	-6.41	1.32	1.45
2	E	1214	DKT	CA1-N	-6.41	1.32	1.45
2	D	1214	DKT	CA1-N	-6.41	1.32	1.45
2	C	1214	DKT	CA1-N	-6.37	1.32	1.45
2	F	1214	DKT	CA1-N	-6.36	1.32	1.45
2	D	1214	DKT	OC2-CC2	-6.16	1.32	1.45
2	B	1214	DKT	OC2-CC2	-6.16	1.32	1.45
2	E	1214	DKT	OC2-CC2	-6.14	1.32	1.45
2	F	1214	DKT	OC2-CC2	-6.13	1.32	1.45
2	A	1214	DKT	OC2-CC2	-6.13	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1214	DKT	OC2-CC2	-6.10	1.32	1.45
2	B	1214	DKT	CA2-N1	-6.07	1.33	1.45
2	A	1214	DKT	CA2-N1	-6.06	1.33	1.45
2	E	1214	DKT	CA2-N1	-6.06	1.33	1.45
2	C	1214	DKT	CA2-N1	-6.05	1.33	1.45
2	F	1214	DKT	CA2-N1	-6.05	1.33	1.45
2	D	1214	DKT	CA2-N1	-6.04	1.33	1.45
2	A	1214	DKT	O2-C8	-5.64	1.12	1.23
2	E	1214	DKT	O2-C8	-5.61	1.12	1.23
2	B	1214	DKT	O2-C8	-5.60	1.12	1.23
2	F	1214	DKT	O2-C8	-5.60	1.12	1.23
2	D	1214	DKT	O2-C8	-5.60	1.12	1.23
2	C	1214	DKT	O2-C8	-5.59	1.12	1.23
2	D	1214	DKT	CE1-CD1	-4.44	1.42	1.53
2	C	1214	DKT	CE1-CD1	-4.42	1.42	1.53
2	E	1214	DKT	CE1-CD1	-4.42	1.42	1.53
2	A	1214	DKT	CE1-CD1	-4.42	1.42	1.53
2	B	1214	DKT	CE1-CD1	-4.40	1.42	1.53
2	F	1214	DKT	CE1-CD1	-4.40	1.42	1.53
2	A	1214	DKT	CE6-CD5	-4.24	1.42	1.53
2	F	1214	DKT	CB1-CG1	-4.23	1.46	1.53
2	B	1214	DKT	CE6-CD5	-4.22	1.42	1.53
2	D	1214	DKT	CE6-CD5	-4.22	1.42	1.53
2	F	1214	DKT	CE6-CD5	-4.21	1.42	1.53
2	B	1214	DKT	CB1-CG1	-4.21	1.46	1.53
2	C	1214	DKT	CE6-CD5	-4.20	1.42	1.53
2	E	1214	DKT	CE6-CD5	-4.20	1.42	1.53
2	A	1214	DKT	CB1-CG1	-4.19	1.46	1.53
2	E	1214	DKT	CB1-CG1	-4.18	1.46	1.53
2	D	1214	DKT	CB1-CG1	-4.17	1.46	1.53
2	C	1214	DKT	CB1-CG1	-4.16	1.46	1.53
2	A	1214	DKT	CE2-CD2	-4.14	1.42	1.53
2	D	1214	DKT	CE2-CD2	-4.12	1.42	1.53
2	F	1214	DKT	CE2-CD2	-4.12	1.42	1.53
2	E	1214	DKT	CE2-CD2	-4.10	1.42	1.53
2	B	1214	DKT	CA3-C9	-4.08	1.42	1.52
2	C	1214	DKT	CE2-CD2	-4.08	1.43	1.53
2	A	1214	DKT	CA3-C9	-4.07	1.42	1.52
2	B	1214	DKT	CE2-CD2	-4.06	1.43	1.53
2	C	1214	DKT	CA3-C9	-4.05	1.42	1.52
2	E	1214	DKT	CA3-C9	-4.05	1.42	1.52
2	F	1214	DKT	CA3-C9	-4.04	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1214	DKT	CA3-C9	-4.03	1.42	1.52
2	A	1214	DKT	CE7-CD6	-3.71	1.43	1.53
2	E	1214	DKT	CE7-CD6	-3.71	1.43	1.53
2	D	1214	DKT	CE7-CD6	-3.70	1.43	1.53
2	F	1214	DKT	CE7-CD6	-3.70	1.43	1.53
2	C	1214	DKT	CE7-CD6	-3.69	1.43	1.53
2	B	1214	DKT	CE7-CD6	-3.69	1.43	1.53
2	E	1214	DKT	CD5-CG4	-3.66	1.41	1.52
2	B	1214	DKT	CD5-CG4	-3.66	1.41	1.52
2	C	1214	DKT	CD5-CG4	-3.66	1.41	1.52
2	D	1214	DKT	CD5-CG4	-3.64	1.42	1.52
2	F	1214	DKT	CD5-CG4	-3.64	1.42	1.52
2	A	1214	DKT	CD5-CG4	-3.63	1.42	1.52
2	D	1214	DKT	C9-N3	-3.38	1.26	1.34
2	E	1214	DKT	C9-N3	-3.38	1.26	1.34
2	D	1214	DKT	CD2-CG1	-3.38	1.42	1.52
2	C	1214	DKT	C9-N3	-3.38	1.26	1.34
2	A	1214	DKT	CD2-CG1	-3.37	1.42	1.52
2	A	1214	DKT	C9-N3	-3.37	1.26	1.34
2	F	1214	DKT	C9-N3	-3.37	1.26	1.34
2	C	1214	DKT	CD1-CG1	-3.37	1.42	1.52
2	B	1214	DKT	CD2-CG1	-3.37	1.42	1.52
2	E	1214	DKT	CD2-CG1	-3.36	1.42	1.52
2	C	1214	DKT	CD2-CG1	-3.36	1.42	1.52
2	F	1214	DKT	CD1-CG1	-3.35	1.42	1.52
2	D	1214	DKT	CD1-CG1	-3.35	1.42	1.52
2	A	1214	DKT	CD1-CG1	-3.34	1.42	1.52
2	E	1214	DKT	CD1-CG1	-3.34	1.42	1.52
2	F	1214	DKT	CD2-CG1	-3.34	1.42	1.52
2	B	1214	DKT	C9-N3	-3.34	1.26	1.34
2	B	1214	DKT	CD1-CG1	-3.34	1.42	1.52
2	B	1214	DKT	CD6-CG4	-3.10	1.43	1.52
2	D	1214	DKT	CD6-CG4	-3.09	1.43	1.52
2	A	1214	DKT	CD6-CG4	-3.06	1.43	1.52
2	E	1214	DKT	CD6-CG4	-3.06	1.43	1.52
2	F	1214	DKT	CD6-CG4	-3.06	1.43	1.52
2	C	1214	DKT	CD6-CG4	-3.06	1.43	1.52
2	C	1214	DKT	CZ1-CE2	-2.60	1.42	1.51
2	B	1214	DKT	CZ1-CE2	-2.60	1.42	1.51
2	E	1214	DKT	CZ1-CE2	-2.59	1.42	1.51
2	A	1214	DKT	CA2-C8	2.59	1.59	1.52
2	A	1214	DKT	CZ1-CE2	-2.58	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1214	DKT	CZ1-CE2	-2.58	1.42	1.51
2	E	1214	DKT	CA2-C8	2.57	1.59	1.52
2	F	1214	DKT	CZ1-CE2	-2.57	1.42	1.51
2	C	1214	DKT	CA2-C8	2.56	1.59	1.52
2	B	1214	DKT	CA2-C8	2.55	1.59	1.52
2	F	1214	DKT	CA2-C8	2.55	1.59	1.52
2	D	1214	DKT	CA2-C8	2.53	1.59	1.52
2	B	1214	DKT	CZ1-CE1	-2.51	1.42	1.51
2	F	1214	DKT	CZ1-CE1	-2.50	1.42	1.51
2	D	1214	DKT	CZ1-CE1	-2.50	1.42	1.51
2	E	1214	DKT	CZ1-CE1	-2.50	1.42	1.51
2	A	1214	DKT	CZ1-CE1	-2.50	1.42	1.51
2	C	1214	DKT	CZ1-CE1	-2.48	1.42	1.51
2	F	1214	DKT	CZ3-CE6	-2.31	1.43	1.51
2	C	1214	DKT	CZ3-CE6	-2.31	1.43	1.51
2	E	1214	DKT	CZ3-CE6	-2.31	1.43	1.51
2	D	1214	DKT	CZ3-CE6	-2.30	1.43	1.51
2	A	1214	DKT	CZ3-CE6	-2.30	1.43	1.51
2	C	1214	DKT	CZ3-CE7	-2.29	1.43	1.51
2	B	1214	DKT	CZ3-CE6	-2.29	1.43	1.51
2	B	1214	DKT	CZ3-CE7	-2.29	1.43	1.51
2	E	1214	DKT	CZ3-CE7	-2.28	1.43	1.51
2	F	1214	DKT	CZ3-CE7	-2.28	1.43	1.51
2	D	1214	DKT	CZ3-CE7	-2.27	1.43	1.51
2	A	1214	DKT	CZ3-CE7	-2.27	1.43	1.51

All (228) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1214	DKT	CG1-CB1-CA1	20.45	142.02	114.52
2	F	1214	DKT	CG1-CB1-CA1	20.44	142.00	114.52
2	B	1214	DKT	CG1-CB1-CA1	20.42	141.98	114.52
2	E	1214	DKT	CG1-CB1-CA1	20.42	141.98	114.52
2	D	1214	DKT	CG1-CB1-CA1	20.42	141.97	114.52
2	C	1214	DKT	CG1-CB1-CA1	20.40	141.95	114.52
2	B	1214	DKT	CB2-CA2-N1	12.78	136.22	110.91
2	E	1214	DKT	CB2-CA2-N1	12.77	136.19	110.91
2	C	1214	DKT	CB2-CA2-N1	12.76	136.17	110.91
2	D	1214	DKT	CB2-CA2-N1	12.76	136.17	110.91
2	A	1214	DKT	CB2-CA2-N1	12.75	136.16	110.91
2	F	1214	DKT	CB2-CA2-N1	12.75	136.15	110.91
2	B	1214	DKT	CC2-OC2-CC1	11.76	142.40	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1214	DKT	CC2-OC2-CC1	11.75	142.38	115.93
2	D	1214	DKT	CC2-OC2-CC1	11.73	142.35	115.93
2	E	1214	DKT	CC2-OC2-CC1	11.73	142.35	115.93
2	F	1214	DKT	CC2-OC2-CC1	11.73	142.33	115.93
2	C	1214	DKT	CC2-OC2-CC1	11.71	142.29	115.93
2	D	1214	DKT	CA2-N1-C6	10.93	140.40	122.00
2	B	1214	DKT	CA2-N1-C6	10.93	140.38	122.00
2	E	1214	DKT	CA2-N1-C6	10.92	140.38	122.00
2	A	1214	DKT	CA2-N1-C6	10.92	140.37	122.00
2	C	1214	DKT	CA2-N1-C6	10.91	140.36	122.00
2	F	1214	DKT	CA2-N1-C6	10.90	140.34	122.00
2	D	1214	DKT	CA2-C8-N2	10.49	139.01	116.63
2	F	1214	DKT	CA2-C8-N2	10.49	139.00	116.63
2	B	1214	DKT	CA2-C8-N2	10.49	139.00	116.63
2	E	1214	DKT	CA2-C8-N2	10.49	139.00	116.63
2	C	1214	DKT	CA2-C8-N2	10.48	138.99	116.63
2	A	1214	DKT	CA2-C8-N2	10.47	138.96	116.63
2	D	1214	DKT	OC2-CC2-CC3	10.29	134.37	109.40
2	E	1214	DKT	OC2-CC2-CC3	10.29	134.37	109.40
2	C	1214	DKT	OC2-CC2-CC3	10.29	134.37	109.40
2	A	1214	DKT	OC2-CC2-CC3	10.29	134.36	109.40
2	B	1214	DKT	OC2-CC2-CC3	10.28	134.34	109.40
2	F	1214	DKT	OC2-CC2-CC3	10.28	134.33	109.40
2	F	1214	DKT	CA3-N2-C8	9.47	141.99	121.65
2	D	1214	DKT	CA3-N2-C8	9.46	141.99	121.65
2	E	1214	DKT	CA3-N2-C8	9.45	141.96	121.65
2	A	1214	DKT	CA3-N2-C8	9.44	141.93	121.65
2	C	1214	DKT	CA3-N2-C8	9.44	141.93	121.65
2	B	1214	DKT	CA3-N2-C8	9.43	141.92	121.65
2	B	1214	DKT	CB1-CG1-CD1	9.32	133.40	111.71
2	C	1214	DKT	CB1-CG1-CD1	9.32	133.40	111.71
2	F	1214	DKT	CB1-CG1-CD1	9.32	133.39	111.71
2	D	1214	DKT	CB1-CG1-CD1	9.31	133.38	111.71
2	E	1214	DKT	CB1-CG1-CD1	9.31	133.38	111.71
2	A	1214	DKT	CB1-CG1-CD1	9.31	133.36	111.71
2	B	1214	DKT	CA1-N-CC1	7.87	140.51	120.93
2	A	1214	DKT	CA1-N-CC1	7.87	140.51	120.93
2	F	1214	DKT	CA1-N-CC1	7.87	140.50	120.93
2	E	1214	DKT	CA1-N-CC1	7.86	140.50	120.93
2	D	1214	DKT	CA1-N-CC1	7.86	140.49	120.93
2	C	1214	DKT	CA1-N-CC1	7.86	140.48	120.93
2	B	1214	DKT	CA3-C9-N3	7.35	132.31	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1214	DKT	CA3-C9-N3	7.33	132.27	116.63
2	D	1214	DKT	CA3-C9-N3	7.33	132.27	116.63
2	A	1214	DKT	CA3-C9-N3	7.33	132.26	116.63
2	E	1214	DKT	CA3-C9-N3	7.33	132.26	116.63
2	F	1214	DKT	CA3-C9-N3	7.32	132.24	116.63
2	C	1214	DKT	O3-C9-CA3	-7.03	105.75	120.48
2	E	1214	DKT	O3-C9-CA3	-7.02	105.77	120.48
2	B	1214	DKT	O3-C9-CA3	-7.01	105.79	120.48
2	D	1214	DKT	O3-C9-CA3	-7.01	105.79	120.48
2	F	1214	DKT	O3-C9-CA3	-7.01	105.80	120.48
2	A	1214	DKT	O3-C9-CA3	-7.01	105.80	120.48
2	F	1214	DKT	O2-C8-N2	-6.31	111.66	122.96
2	D	1214	DKT	O2-C8-N2	-6.29	111.70	122.96
2	E	1214	DKT	O2-C8-N2	-6.28	111.71	122.96
2	C	1214	DKT	O2-C8-N2	-6.28	111.71	122.96
2	B	1214	DKT	O2-C8-N2	-6.28	111.72	122.96
2	A	1214	DKT	O2-C8-N2	-6.24	111.78	122.96
2	B	1214	DKT	CA4-N3-C9	5.49	133.45	121.65
2	D	1214	DKT	CA4-N3-C9	5.49	133.44	121.65
2	A	1214	DKT	CA4-N3-C9	5.47	133.41	121.65
2	E	1214	DKT	CA4-N3-C9	5.47	133.40	121.65
2	F	1214	DKT	CA4-N3-C9	5.46	133.39	121.65
2	C	1214	DKT	CA4-N3-C9	5.46	133.37	121.65
2	A	1214	DKT	O2-C8-CA2	-5.36	109.26	120.48
2	B	1214	DKT	O2-C8-CA2	-5.35	109.28	120.48
2	D	1214	DKT	O2-C8-CA2	-5.34	109.29	120.48
2	E	1214	DKT	O2-C8-CA2	-5.34	109.29	120.48
2	C	1214	DKT	O2-C8-CA2	-5.34	109.30	120.48
2	F	1214	DKT	O2-C8-CA2	-5.32	109.33	120.48
2	F	1214	DKT	O12-CC1-N	-4.96	116.73	124.86
2	A	1214	DKT	O12-CC1-N	-4.96	116.73	124.86
2	E	1214	DKT	O12-CC1-N	-4.96	116.73	124.86
2	D	1214	DKT	O12-CC1-N	-4.95	116.75	124.86
2	B	1214	DKT	O12-CC1-N	-4.95	116.76	124.86
2	C	1214	DKT	O12-CC1-N	-4.94	116.76	124.86
2	B	1214	DKT	CE6-CD5-CG4	4.30	121.13	112.08
2	A	1214	DKT	CE6-CD5-CG4	4.29	121.12	112.08
2	F	1214	DKT	CZ3-CE6-CD5	4.29	120.24	111.42
2	C	1214	DKT	CE6-CD5-CG4	4.28	121.10	112.08
2	A	1214	DKT	CZ3-CE6-CD5	4.28	120.22	111.42
2	C	1214	DKT	CZ3-CE6-CD5	4.28	120.22	111.42
2	E	1214	DKT	CE6-CD5-CG4	4.28	121.09	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1214	DKT	CZ3-CE6-CD5	4.28	120.21	111.42
2	D	1214	DKT	CE6-CD5-CG4	4.27	121.08	112.08
2	E	1214	DKT	CZ3-CE6-CD5	4.27	120.20	111.42
2	F	1214	DKT	CE6-CD5-CG4	4.26	121.05	112.08
2	B	1214	DKT	CZ3-CE6-CD5	4.26	120.17	111.42
2	D	1214	DKT	CZ1-CE2-CD2	4.22	120.10	111.42
2	F	1214	DKT	CZ1-CE2-CD2	4.22	120.08	111.42
2	F	1214	DKT	CE1-CD1-CG1	4.21	120.95	112.08
2	E	1214	DKT	CZ1-CE2-CD2	4.21	120.07	111.42
2	A	1214	DKT	CZ1-CE2-CD2	4.20	120.06	111.42
2	B	1214	DKT	CZ1-CE2-CD2	4.20	120.06	111.42
2	C	1214	DKT	CE1-CD1-CG1	4.20	120.93	112.08
2	B	1214	DKT	CE1-CD1-CG1	4.20	120.92	112.08
2	C	1214	DKT	CZ1-CE2-CD2	4.20	120.05	111.42
2	D	1214	DKT	CE1-CD1-CG1	4.19	120.91	112.08
2	E	1214	DKT	CE1-CD1-CG1	4.19	120.91	112.08
2	A	1214	DKT	CE1-CD1-CG1	4.18	120.88	112.08
2	D	1214	DKT	CE7-CD6-CG4	4.17	120.87	112.08
2	B	1214	DKT	CE7-CD6-CG4	4.16	120.85	112.08
2	F	1214	DKT	CE7-CD6-CG4	4.16	120.84	112.08
2	E	1214	DKT	CE7-CD6-CG4	4.16	120.83	112.08
2	A	1214	DKT	CE7-CD6-CG4	4.15	120.83	112.08
2	C	1214	DKT	CE7-CD6-CG4	4.15	120.82	112.08
2	D	1214	DKT	CB4-CG4-CD6	4.11	121.27	111.71
2	B	1214	DKT	CB4-CG4-CD6	4.09	121.23	111.71
2	F	1214	DKT	CB4-CG4-CD6	4.09	121.23	111.71
2	E	1214	DKT	CB4-CG4-CD6	4.09	121.22	111.71
2	A	1214	DKT	CB4-CG4-CD6	4.08	121.21	111.71
2	C	1214	DKT	CB4-CG4-CD6	4.08	121.20	111.71
2	C	1214	DKT	CD2-CG1-CD1	4.02	119.12	109.29
2	D	1214	DKT	CZ1-CE1-CD1	4.02	119.68	111.42
2	D	1214	DKT	CD2-CG1-CD1	4.02	119.11	109.29
2	A	1214	DKT	CD2-CG1-CD1	4.02	119.10	109.29
2	A	1214	DKT	CZ1-CE1-CD1	4.01	119.67	111.42
2	E	1214	DKT	CD2-CG1-CD1	4.01	119.10	109.29
2	B	1214	DKT	CD2-CG1-CD1	4.01	119.08	109.29
2	E	1214	DKT	CZ1-CE1-CD1	4.01	119.66	111.42
2	B	1214	DKT	CZ1-CE1-CD1	4.01	119.65	111.42
2	F	1214	DKT	CD2-CG1-CD1	4.00	119.07	109.29
2	F	1214	DKT	CZ1-CE1-CD1	4.00	119.63	111.42
2	C	1214	DKT	CZ1-CE1-CD1	4.00	119.63	111.42
2	A	1214	DKT	CZ3-CE7-CD6	3.93	119.49	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1214	DKT	CZ3-CE7-CD6	3.92	119.48	111.42
2	E	1214	DKT	CZ3-CE7-CD6	3.91	119.46	111.42
2	D	1214	DKT	CD6-CG4-CD5	3.91	118.84	109.29
2	F	1214	DKT	CD6-CG4-CD5	3.91	118.84	109.29
2	B	1214	DKT	CZ3-CE7-CD6	3.91	119.45	111.42
2	E	1214	DKT	CD6-CG4-CD5	3.90	118.83	109.29
2	B	1214	DKT	CD6-CG4-CD5	3.90	118.83	109.29
2	F	1214	DKT	CZ3-CE7-CD6	3.90	119.44	111.42
2	C	1214	DKT	CD6-CG4-CD5	3.90	118.81	109.29
2	A	1214	DKT	CD6-CG4-CD5	3.90	118.81	109.29
2	D	1214	DKT	CZ3-CE7-CD6	3.89	119.42	111.42
2	A	1214	DKT	CE2-CD2-CG1	3.88	120.25	112.08
2	F	1214	DKT	CE2-CD2-CG1	3.86	120.21	112.08
2	E	1214	DKT	CE2-CD2-CG1	3.86	120.21	112.08
2	B	1214	DKT	CE2-CD2-CG1	3.86	120.21	112.08
2	D	1214	DKT	CE2-CD2-CG1	3.86	120.20	112.08
2	C	1214	DKT	CE2-CD2-CG1	3.86	120.20	112.08
2	F	1214	DKT	OC2-CC1-N	3.79	118.56	110.45
2	D	1214	DKT	OC2-CC1-N	3.79	118.55	110.45
2	E	1214	DKT	OC2-CC1-N	3.77	118.52	110.45
2	A	1214	DKT	OC2-CC1-N	3.77	118.52	110.45
2	C	1214	DKT	OC2-CC1-N	3.77	118.51	110.45
2	B	1214	DKT	OC2-CC1-N	3.75	118.48	110.45
2	C	1214	DKT	CB4-CG4-CD5	3.56	119.98	111.71
2	A	1214	DKT	CB4-CG4-CD5	3.55	119.98	111.71
2	E	1214	DKT	CB4-CG4-CD5	3.54	119.95	111.71
2	B	1214	DKT	CB4-CG4-CD5	3.54	119.94	111.71
2	F	1214	DKT	CB4-CG4-CD5	3.54	119.94	111.71
2	D	1214	DKT	CB4-CG4-CD5	3.52	119.89	111.71
2	B	1214	DKT	CB3-CA3-N2	-3.45	104.08	110.91
2	C	1214	DKT	CB3-CA3-N2	-3.45	104.08	110.91
2	E	1214	DKT	CB3-CA3-N2	-3.43	104.12	110.91
2	A	1214	DKT	CB3-CA3-N2	-3.42	104.14	110.91
2	F	1214	DKT	CB3-CA3-N2	-3.41	104.16	110.91
2	D	1214	DKT	CB3-CA3-N2	-3.41	104.16	110.91
2	D	1214	DKT	CC2-CC3-C2	-3.30	113.04	120.64
2	F	1214	DKT	CC2-CC3-C2	-3.30	113.04	120.64
2	B	1214	DKT	CC2-CC3-C2	-3.29	113.05	120.64
2	C	1214	DKT	CC2-CC3-C2	-3.29	113.06	120.64
2	A	1214	DKT	CC2-CC3-C2	-3.29	113.06	120.64
2	E	1214	DKT	CC2-CC3-C2	-3.29	113.06	120.64
2	B	1214	DKT	C8-CA2-N1	-3.27	102.25	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1214	DKT	C8-CA2-N1	-3.26	102.29	111.11
2	F	1214	DKT	C8-CA2-N1	-3.26	102.30	111.11
2	D	1214	DKT	C8-CA2-N1	-3.25	102.31	111.11
2	A	1214	DKT	C8-CA2-N1	-3.25	102.31	111.11
2	C	1214	DKT	C8-CA2-N1	-3.25	102.32	111.11
2	C	1214	DKT	O-C6-N1	3.20	128.72	123.09
2	D	1214	DKT	O-C6-N1	3.19	128.71	123.09
2	B	1214	DKT	O-C6-N1	3.17	128.68	123.09
2	E	1214	DKT	O-C6-N1	3.17	128.68	123.09
2	A	1214	DKT	O-C6-N1	3.16	128.66	123.09
2	F	1214	DKT	O-C6-N1	3.15	128.65	123.09
2	B	1214	DKT	CE2-CZ1-CE1	2.99	120.07	111.19
2	C	1214	DKT	CE2-CZ1-CE1	2.99	120.07	111.19
2	E	1214	DKT	CE2-CZ1-CE1	2.99	120.06	111.19
2	F	1214	DKT	CE2-CZ1-CE1	2.98	120.05	111.19
2	A	1214	DKT	CE2-CZ1-CE1	2.98	120.03	111.19
2	D	1214	DKT	CE2-CZ1-CE1	2.97	120.00	111.19
2	D	1214	DKT	CE7-CZ3-CE6	2.83	119.59	111.19
2	F	1214	DKT	CE7-CZ3-CE6	2.83	119.58	111.19
2	E	1214	DKT	CE7-CZ3-CE6	2.83	119.58	111.19
2	B	1214	DKT	CE7-CZ3-CE6	2.82	119.57	111.19
2	C	1214	DKT	CE7-CZ3-CE6	2.82	119.56	111.19
2	A	1214	DKT	CE7-CZ3-CE6	2.81	119.53	111.19
2	C	1214	DKT	CC2-CC3-C5	2.59	126.61	120.64
2	F	1214	DKT	CC2-CC3-C5	2.59	126.61	120.64
2	D	1214	DKT	CC2-CC3-C5	2.59	126.61	120.64
2	A	1214	DKT	CC2-CC3-C5	2.59	126.61	120.64
2	E	1214	DKT	CC2-CC3-C5	2.58	126.60	120.64
2	B	1214	DKT	CC2-CC3-C5	2.58	126.58	120.64
2	B	1214	DKT	CB1-CA1-N	2.36	115.90	110.58
2	C	1214	DKT	CB1-CA1-N	2.35	115.88	110.58
2	E	1214	DKT	CB1-CA1-N	2.33	115.85	110.58
2	F	1214	DKT	CB1-CA1-N	2.33	115.84	110.58
2	A	1214	DKT	CB1-CA1-N	2.32	115.82	110.58
2	D	1214	DKT	CB1-CA1-N	2.32	115.81	110.58
2	F	1214	DKT	OXT-C10-CA4	2.16	120.83	113.51
2	B	1214	DKT	OXT-C10-CA4	2.15	120.80	113.51
2	D	1214	DKT	OXT-C10-CA4	2.15	120.80	113.51
2	A	1214	DKT	OXT-C10-CA4	2.15	120.80	113.51
2	E	1214	DKT	OXT-C10-CA4	2.15	120.77	113.51
2	C	1214	DKT	CB1-CG1-CD2	-2.14	106.74	111.71
2	C	1214	DKT	OXT-C10-CA4	2.13	120.72	113.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1214	DKT	CB1-CG1-CD2	-2.12	106.77	111.71
2	A	1214	DKT	CB1-CG1-CD2	-2.12	106.77	111.71
2	E	1214	DKT	CB1-CG1-CD2	-2.12	106.77	111.71
2	B	1214	DKT	CB1-CG1-CD2	-2.12	106.78	111.71
2	F	1214	DKT	CB1-CG1-CD2	-2.11	106.79	111.71

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1214	DKT	CA1
2	B	1214	DKT	CA1
2	C	1214	DKT	CA1
2	D	1214	DKT	CA1
2	E	1214	DKT	CA1
2	F	1214	DKT	CA1

All (162) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1214	DKT	N-CC1-OC2-CC2
2	A	1214	DKT	O12-CC1-OC2-CC2
2	A	1214	DKT	CC3-CC2-OC2-CC1
2	A	1214	DKT	N-CA1-CB1-CG1
2	A	1214	DKT	C6-C7-CA1-N
2	A	1214	DKT	O-C6-C7-CA1
2	A	1214	DKT	O-C6-C7-O1
2	A	1214	DKT	N1-C6-C7-CA1
2	A	1214	DKT	N1-C6-C7-O1
2	A	1214	DKT	C7-C6-N1-CA2
2	A	1214	DKT	C8-CA2-CB2-CG2
2	B	1214	DKT	N-CC1-OC2-CC2
2	B	1214	DKT	O12-CC1-OC2-CC2
2	B	1214	DKT	CC3-CC2-OC2-CC1
2	B	1214	DKT	N-CA1-CB1-CG1
2	B	1214	DKT	C6-C7-CA1-N
2	B	1214	DKT	O-C6-C7-CA1
2	B	1214	DKT	O-C6-C7-O1
2	B	1214	DKT	N1-C6-C7-CA1
2	B	1214	DKT	N1-C6-C7-O1
2	B	1214	DKT	C7-C6-N1-CA2
2	B	1214	DKT	C8-CA2-CB2-CG2
2	C	1214	DKT	N-CC1-OC2-CC2

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Mol	Chain	Res	Type	Atoms
2	C	1214	DKT	O12-CC1-OC2-CC2
2	C	1214	DKT	CC3-CC2-OC2-CC1
2	C	1214	DKT	N-CA1-CB1-CG1
2	C	1214	DKT	C6-C7-CA1-N
2	C	1214	DKT	O-C6-C7-CA1
2	C	1214	DKT	O-C6-C7-O1
2	C	1214	DKT	N1-C6-C7-CA1
2	C	1214	DKT	N1-C6-C7-O1
2	C	1214	DKT	C7-C6-N1-CA2
2	C	1214	DKT	C8-CA2-CB2-CG2
2	D	1214	DKT	N-CC1-OC2-CC2
2	D	1214	DKT	O12-CC1-OC2-CC2
2	D	1214	DKT	CC3-CC2-OC2-CC1
2	D	1214	DKT	N-CA1-CB1-CG1
2	D	1214	DKT	C6-C7-CA1-N
2	D	1214	DKT	O-C6-C7-CA1
2	D	1214	DKT	O-C6-C7-O1
2	D	1214	DKT	N1-C6-C7-CA1
2	D	1214	DKT	N1-C6-C7-O1
2	D	1214	DKT	C7-C6-N1-CA2
2	D	1214	DKT	C8-CA2-CB2-CG2
2	E	1214	DKT	N-CC1-OC2-CC2
2	E	1214	DKT	O12-CC1-OC2-CC2
2	E	1214	DKT	CC3-CC2-OC2-CC1
2	E	1214	DKT	N-CA1-CB1-CG1
2	E	1214	DKT	C6-C7-CA1-N
2	E	1214	DKT	O-C6-C7-CA1
2	E	1214	DKT	O-C6-C7-O1
2	E	1214	DKT	N1-C6-C7-CA1
2	E	1214	DKT	N1-C6-C7-O1
2	E	1214	DKT	C7-C6-N1-CA2
2	E	1214	DKT	C8-CA2-CB2-CG2
2	F	1214	DKT	N-CC1-OC2-CC2
2	F	1214	DKT	O12-CC1-OC2-CC2
2	F	1214	DKT	CC3-CC2-OC2-CC1
2	F	1214	DKT	N-CA1-CB1-CG1
2	F	1214	DKT	C6-C7-CA1-N
2	F	1214	DKT	O-C6-C7-CA1
2	F	1214	DKT	O-C6-C7-O1
2	F	1214	DKT	N1-C6-C7-CA1
2	F	1214	DKT	N1-C6-C7-O1
2	F	1214	DKT	C7-C6-N1-CA2

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Mol	Chain	Res	Type	Atoms
2	F	1214	DKT	C8-CA2-CB2-CG2
2	A	1214	DKT	N1-CA2-CB2-CG2
2	B	1214	DKT	N1-CA2-CB2-CG2
2	C	1214	DKT	N1-CA2-CB2-CG2
2	D	1214	DKT	N1-CA2-CB2-CG2
2	E	1214	DKT	N1-CA2-CB2-CG2
2	F	1214	DKT	N1-CA2-CB2-CG2
2	A	1214	DKT	NE3-CD3-CG2-CB2
2	B	1214	DKT	NE3-CD3-CG2-CB2
2	C	1214	DKT	NE3-CD3-CG2-CB2
2	D	1214	DKT	NE3-CD3-CG2-CB2
2	E	1214	DKT	NE3-CD3-CG2-CB2
2	F	1214	DKT	NE3-CD3-CG2-CB2
2	A	1214	DKT	OXT-C10-CA4-CB4
2	B	1214	DKT	OXT-C10-CA4-CB4
2	C	1214	DKT	OXT-C10-CA4-CB4
2	D	1214	DKT	OXT-C10-CA4-CB4
2	E	1214	DKT	OXT-C10-CA4-CB4
2	F	1214	DKT	OXT-C10-CA4-CB4
2	A	1214	DKT	CA1-CB1-CG1-CD1
2	A	1214	DKT	CA4-CB4-CG4-CD6
2	B	1214	DKT	CA1-CB1-CG1-CD1
2	B	1214	DKT	CA4-CB4-CG4-CD6
2	C	1214	DKT	CA1-CB1-CG1-CD1
2	C	1214	DKT	CA4-CB4-CG4-CD6
2	D	1214	DKT	CA1-CB1-CG1-CD1
2	D	1214	DKT	CA4-CB4-CG4-CD6
2	E	1214	DKT	CA1-CB1-CG1-CD1
2	E	1214	DKT	CA4-CB4-CG4-CD6
2	F	1214	DKT	CA1-CB1-CG1-CD1
2	F	1214	DKT	CA4-CB4-CG4-CD6
2	A	1214	DKT	OT-C10-CA4-CB4
2	B	1214	DKT	OT-C10-CA4-CB4
2	C	1214	DKT	OT-C10-CA4-CB4
2	D	1214	DKT	OT-C10-CA4-CB4
2	E	1214	DKT	OT-C10-CA4-CB4
2	F	1214	DKT	OT-C10-CA4-CB4
2	A	1214	DKT	CB4-CA4-N3-C9
2	B	1214	DKT	CB4-CA4-N3-C9
2	C	1214	DKT	CB4-CA4-N3-C9
2	D	1214	DKT	CB4-CA4-N3-C9
2	E	1214	DKT	CB4-CA4-N3-C9

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Mol	Chain	Res	Type	Atoms
2	F	1214	DKT	CB4-CA4-N3-C9
2	A	1214	DKT	O2-C8-CA2-CB2
2	B	1214	DKT	O2-C8-CA2-CB2
2	C	1214	DKT	O2-C8-CA2-CB2
2	D	1214	DKT	O2-C8-CA2-CB2
2	E	1214	DKT	O2-C8-CA2-CB2
2	F	1214	DKT	O2-C8-CA2-CB2
2	A	1214	DKT	OT-C10-CA4-N3
2	A	1214	DKT	OXT-C10-CA4-N3
2	B	1214	DKT	OT-C10-CA4-N3
2	B	1214	DKT	OXT-C10-CA4-N3
2	C	1214	DKT	OT-C10-CA4-N3
2	C	1214	DKT	OXT-C10-CA4-N3
2	D	1214	DKT	OT-C10-CA4-N3
2	D	1214	DKT	OXT-C10-CA4-N3
2	E	1214	DKT	OT-C10-CA4-N3
2	E	1214	DKT	OXT-C10-CA4-N3
2	F	1214	DKT	OT-C10-CA4-N3
2	F	1214	DKT	OXT-C10-CA4-N3
2	A	1214	DKT	N2-C8-CA2-CB2
2	B	1214	DKT	N2-C8-CA2-CB2
2	C	1214	DKT	N2-C8-CA2-CB2
2	D	1214	DKT	N2-C8-CA2-CB2
2	E	1214	DKT	N2-C8-CA2-CB2
2	F	1214	DKT	N2-C8-CA2-CB2
2	A	1214	DKT	CG2-CD3-NE3-CZ2
2	B	1214	DKT	CG2-CD3-NE3-CZ2
2	C	1214	DKT	CG2-CD3-NE3-CZ2
2	D	1214	DKT	CG2-CD3-NE3-CZ2
2	E	1214	DKT	CG2-CD3-NE3-CZ2
2	F	1214	DKT	CG2-CD3-NE3-CZ2
2	B	1214	DKT	C7-CA1-CB1-CG1
2	C	1214	DKT	C7-CA1-CB1-CG1
2	D	1214	DKT	C7-CA1-CB1-CG1
2	F	1214	DKT	C7-CA1-CB1-CG1
2	A	1214	DKT	C7-CA1-CB1-CG1
2	E	1214	DKT	C7-CA1-CB1-CG1
2	A	1214	DKT	O1-C7-CA1-CB1
2	B	1214	DKT	O1-C7-CA1-CB1
2	C	1214	DKT	O1-C7-CA1-CB1
2	D	1214	DKT	O1-C7-CA1-CB1
2	E	1214	DKT	O1-C7-CA1-CB1

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Mol	Chain	Res	Type	Atoms
2	F	1214	DKT	O1-C7-CA1-CB1
2	A	1214	DKT	OE5-CD4-CG3-CB3
2	B	1214	DKT	OE5-CD4-CG3-CB3
2	C	1214	DKT	OE5-CD4-CG3-CB3
2	E	1214	DKT	OE5-CD4-CG3-CB3
2	D	1214	DKT	OE4-CD4-CG3-CB3
2	D	1214	DKT	OE5-CD4-CG3-CB3
2	E	1214	DKT	OE4-CD4-CG3-CB3
2	F	1214	DKT	OE5-CD4-CG3-CB3
2	A	1214	DKT	OE4-CD4-CG3-CB3
2	B	1214	DKT	OE4-CD4-CG3-CB3
2	C	1214	DKT	OE4-CD4-CG3-CB3
2	F	1214	DKT	OE4-CD4-CG3-CB3

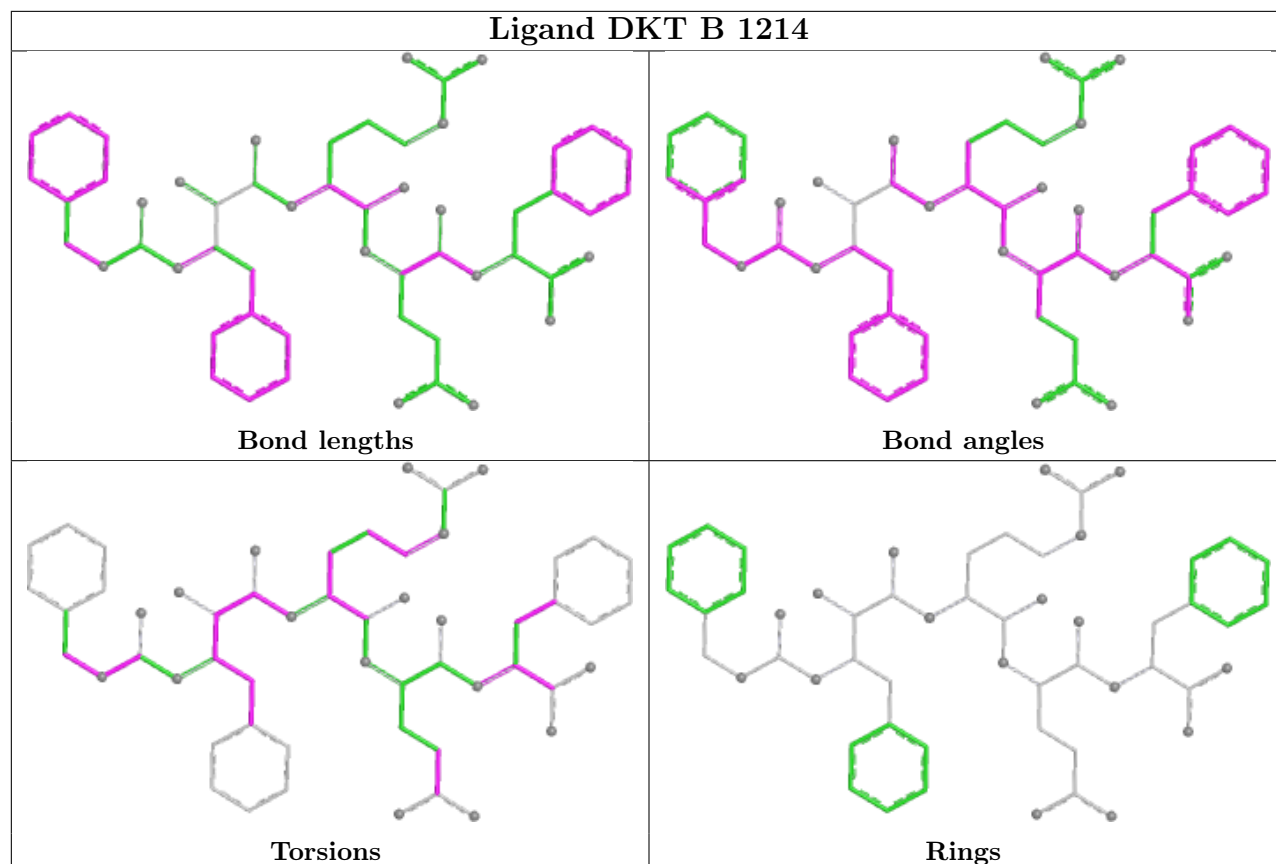
There are no ring outliers.

6 monomers are involved in 72 short contacts:

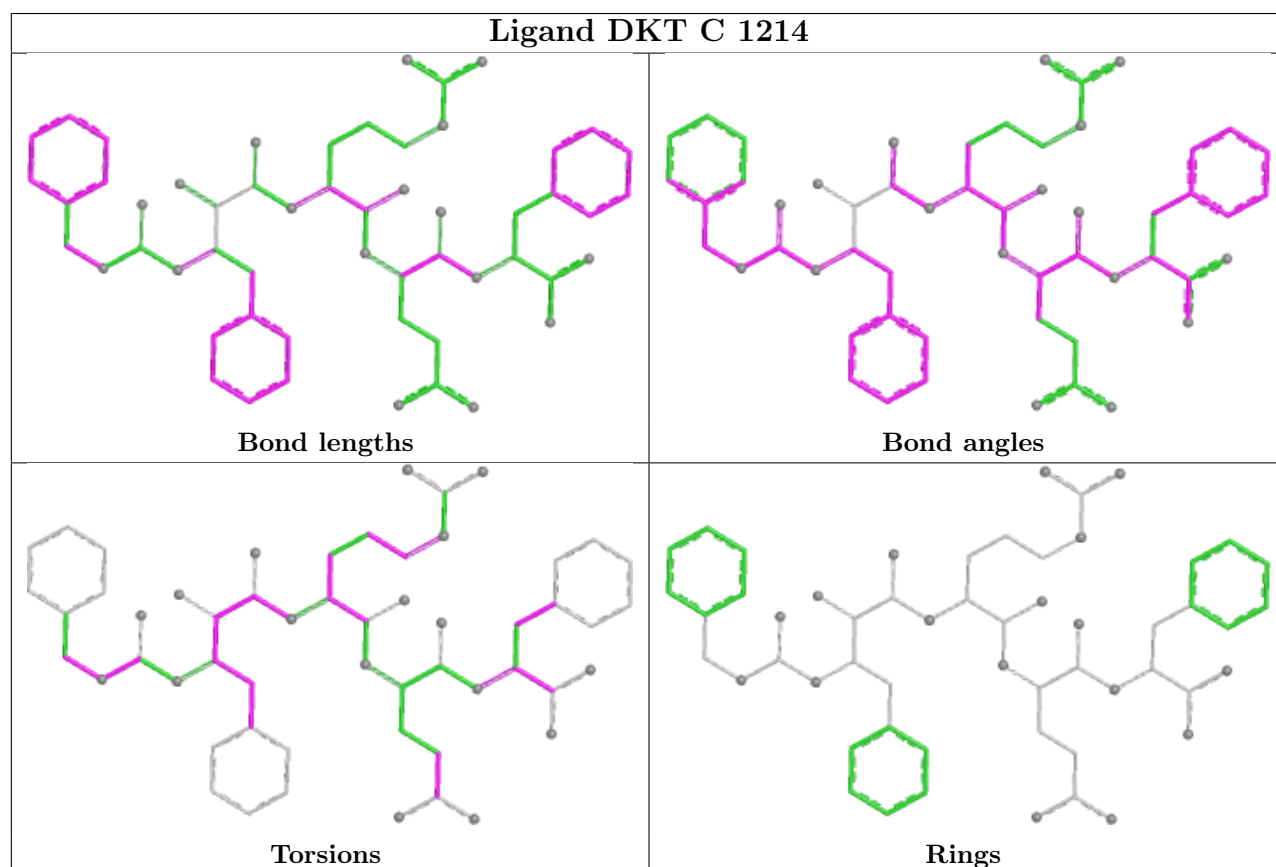
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1214	DKT	7	0
2	C	1214	DKT	8	0
2	F	1214	DKT	11	0
2	D	1214	DKT	8	0
2	E	1214	DKT	18	0
2	A	1214	DKT	20	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

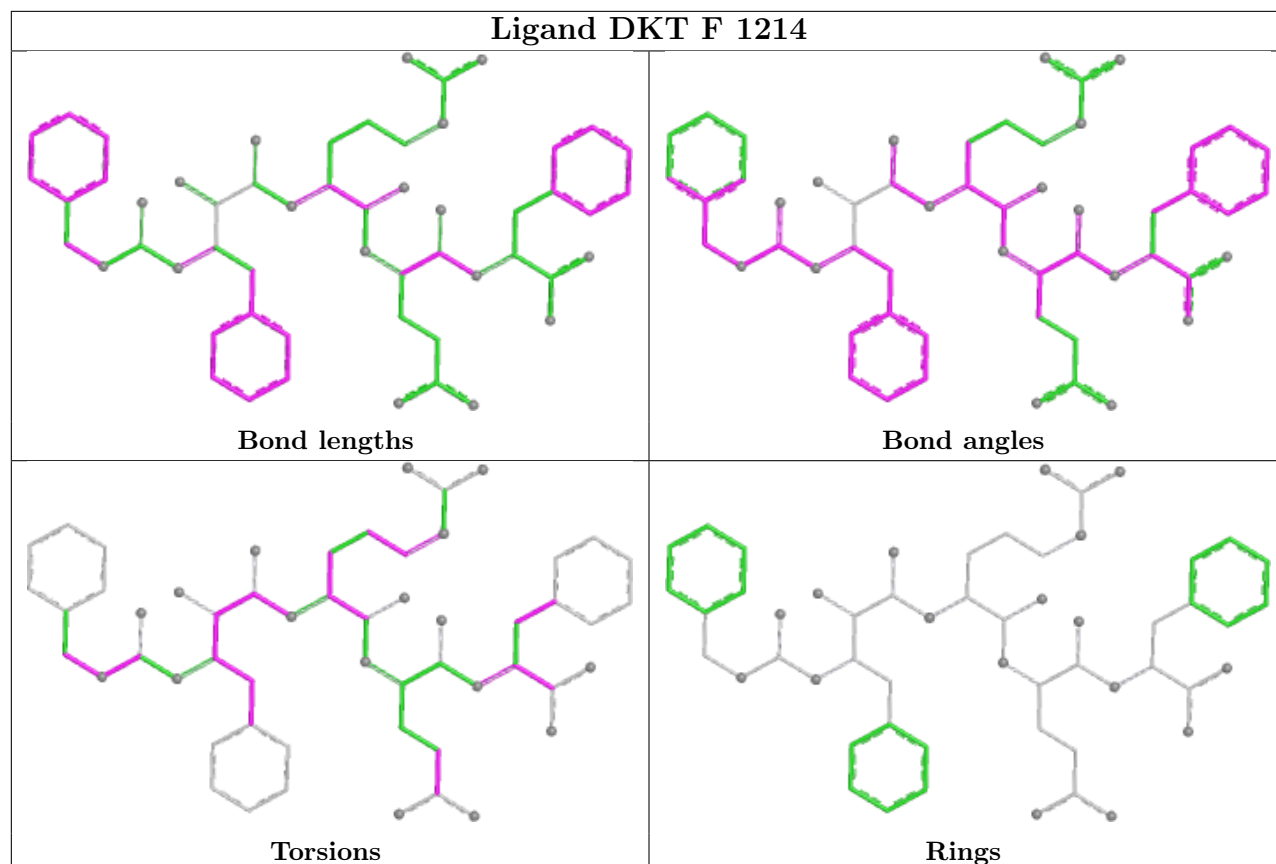
Ligand DKT B 1214



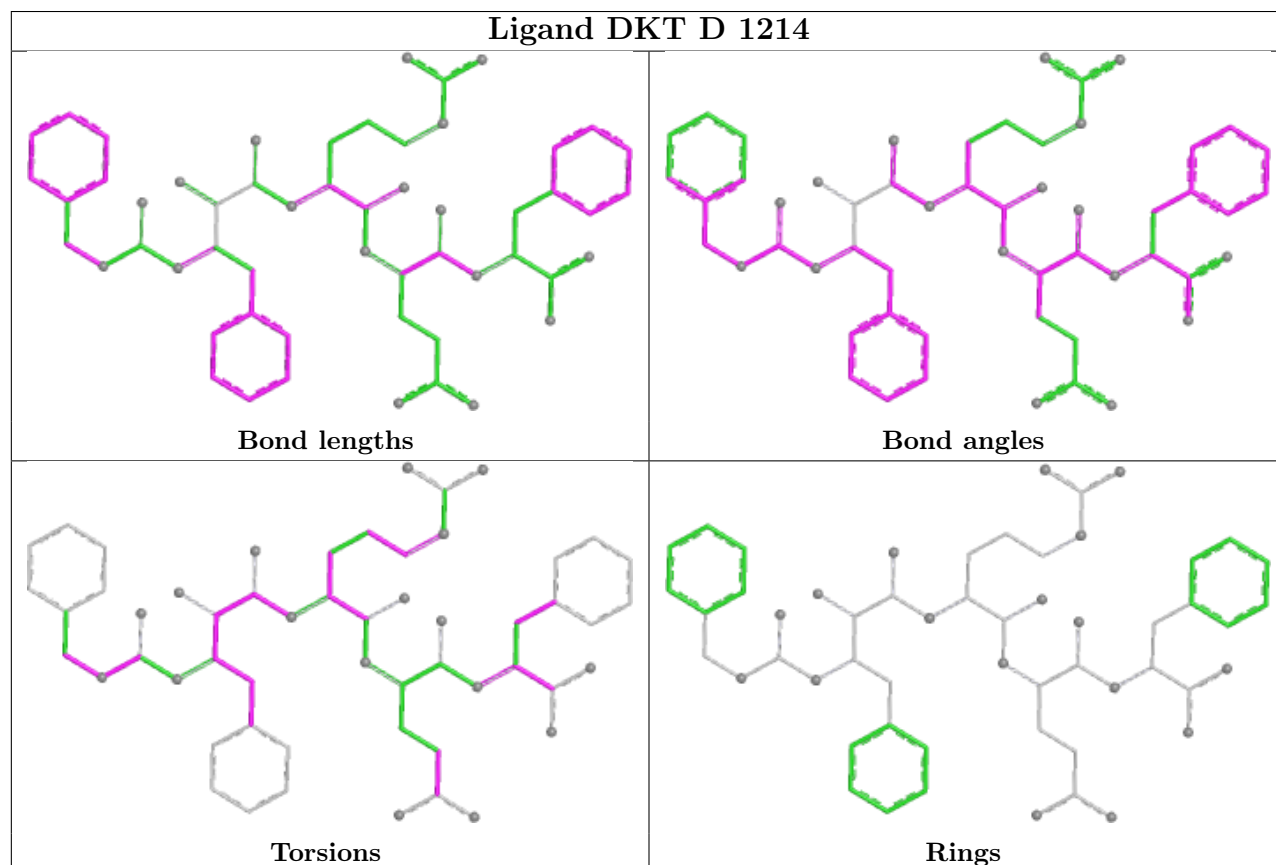
Ligand DKT C 1214



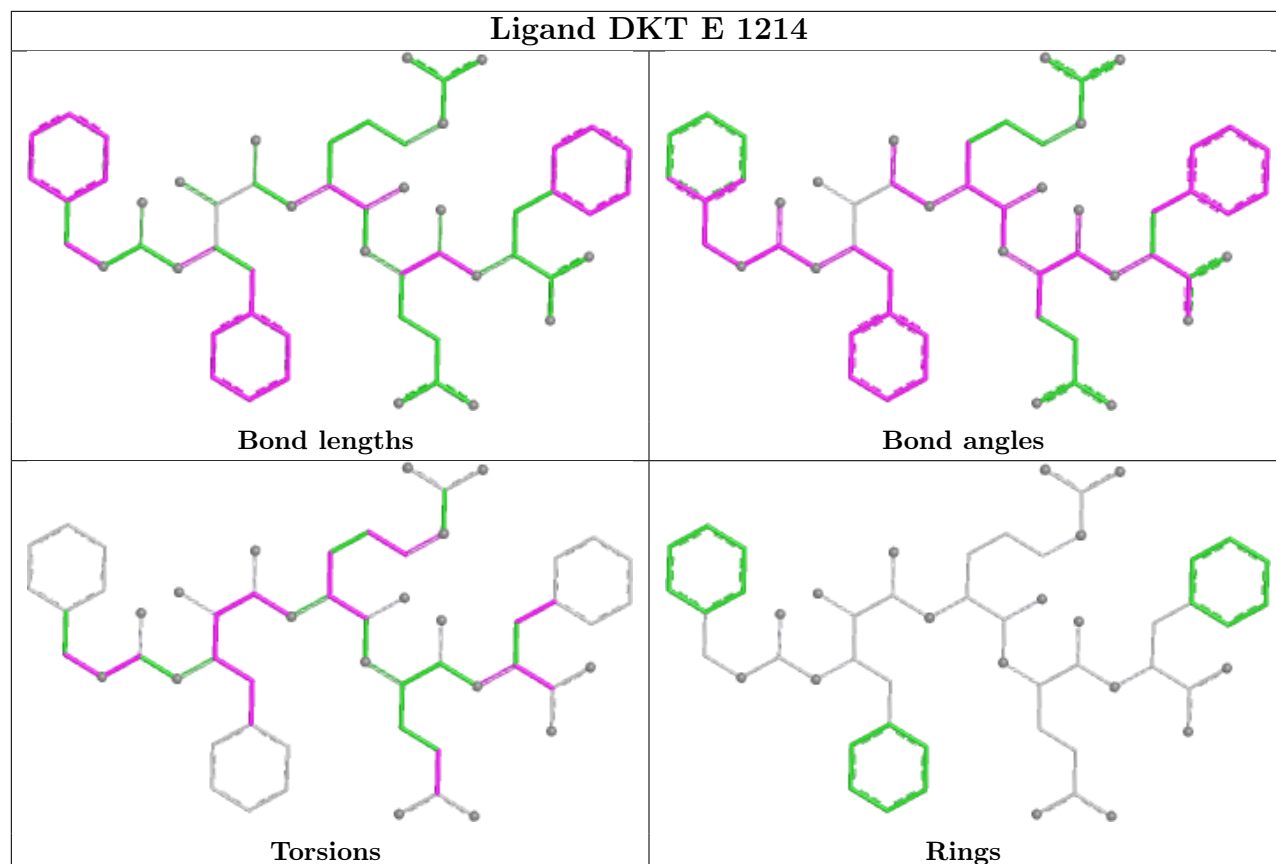
Ligand DKT F 1214



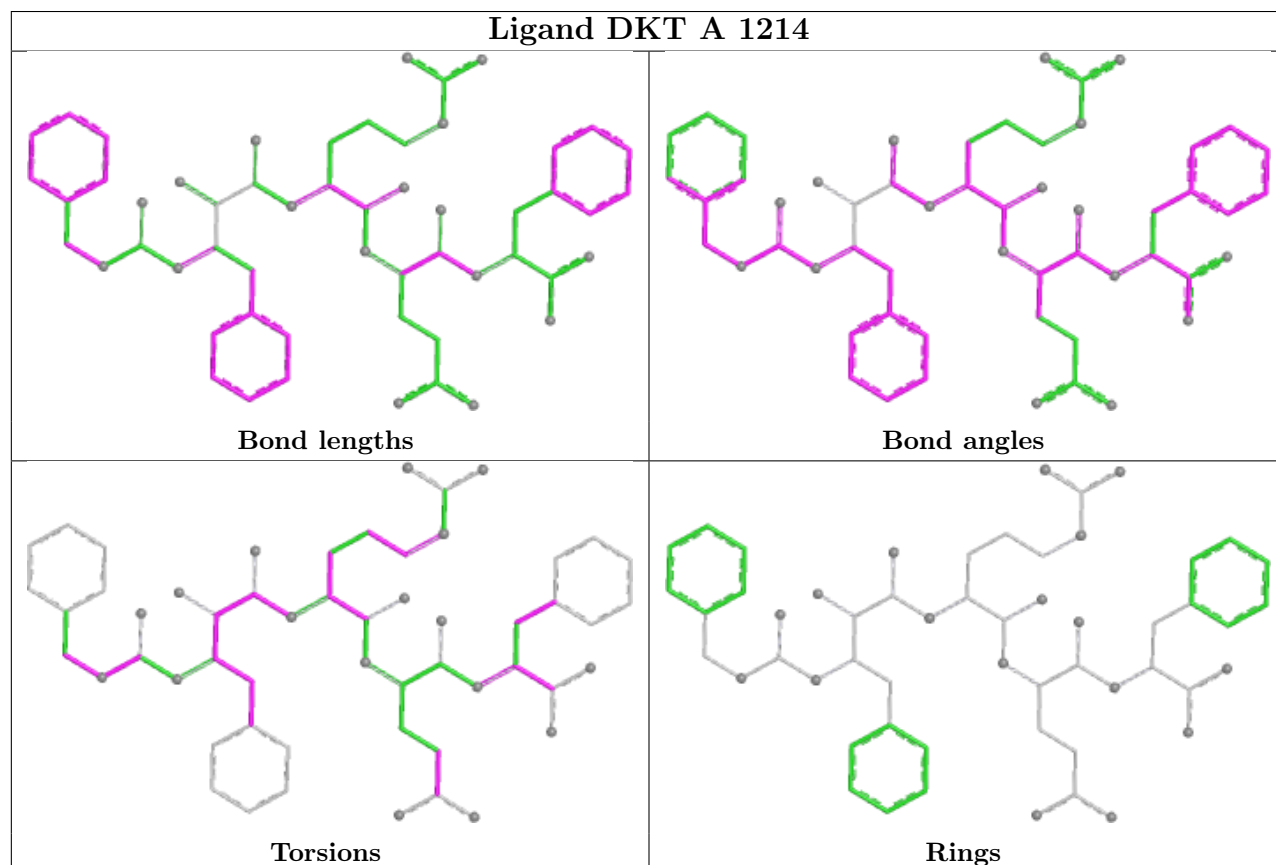
Ligand DKT D 1214



Ligand DKT E 1214



Ligand DKT A 1214



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1023/1071 (95%)	-0.28	18 (1%) 67 65	7, 34, 57, 85	20 (1%)
1	B	1023/1071 (95%)	-0.30	11 (1%) 78 76	7, 34, 57, 85	20 (1%)
1	C	1023/1071 (95%)	-0.13	10 (0%) 79 78	7, 39, 60, 85	20 (1%)
1	D	1023/1071 (95%)	-0.28	10 (0%) 79 78	7, 35, 58, 84	20 (1%)
1	E	1023/1071 (95%)	-0.29	10 (0%) 79 78	7, 35, 58, 83	20 (1%)
1	F	1023/1071 (95%)	-0.18	9 (0%) 81 80	7, 38, 60, 85	20 (1%)
All	All	6138/6426 (95%)	-0.24	68 (1%) 78 76	7, 36, 59, 85	120 (1%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	220	GLY	4.2
1	B	842	GLY	4.1
1	A	562	GLU	4.0
1	C	562	GLU	4.0
1	D	218	ASN	3.9
1	E	219	SER	3.8
1	A	563	ALA	3.6
1	A	329	PHE	3.5
1	E	300	THR	3.4
1	F	1061	ASN	3.3
1	A	842	GLY	3.2
1	B	562	GLU	3.1
1	C	563	ALA	3.0
1	E	705	ALA	3.0
1	A	840	LYS	3.0
1	D	563	ALA	3.0
1	D	300	THR	2.9
1	F	563	ALA	2.9
1	D	329	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	562	GLU	2.8
1	F	840	LYS	2.8
1	E	561	SER	2.7
1	A	716	GLU	2.7
1	E	565	GLU	2.7
1	A	705	ALA	2.6
1	C	88	PRO	2.6
1	D	219	SER	2.6
1	A	708	LYS	2.6
1	C	188	GLY	2.6
1	D	841	GLY	2.6
1	D	683	HIS	2.6
1	C	220	GLY	2.6
1	B	329	PHE	2.5
1	E	39	MET	2.5
1	C	258	ASP	2.5
1	F	564	GLY	2.5
1	F	816	GLY	2.5
1	B	644	ASP	2.5
1	B	88	PRO	2.5
1	D	489	LYS	2.4
1	A	299	ASP	2.4
1	C	187	ASP	2.4
1	A	167	ASN	2.4
1	A	561	SER	2.4
1	E	398	GLU	2.3
1	A	88	PRO	2.3
1	A	218	ASN	2.2
1	F	297	ASN	2.2
1	C	143	ASP	2.2
1	A	297	ASN	2.2
1	B	612	GLY	2.2
1	B	818	GLY	2.2
1	E	329	PHE	2.2
1	A	683	HIS	2.1
1	F	667	ASP	2.1
1	A	401	GLU	2.1
1	B	218	ASN	2.1
1	A	143	ASP	2.1
1	F	329	PHE	2.1
1	E	563	ALA	2.1
1	C	144	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	772	ASP	2.1
1	B	563	ALA	2.1
1	C	142	PRO	2.0
1	A	435	THR	2.0
1	D	626	THR	2.0
1	F	300	THR	2.0
1	B	1061	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

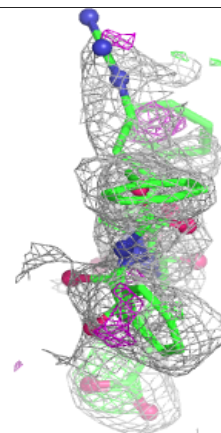
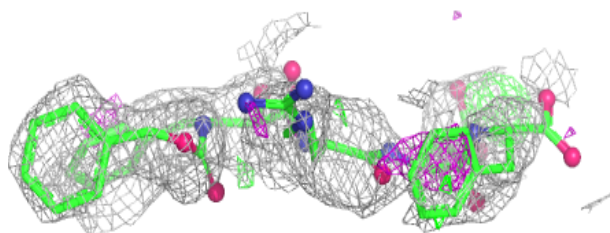
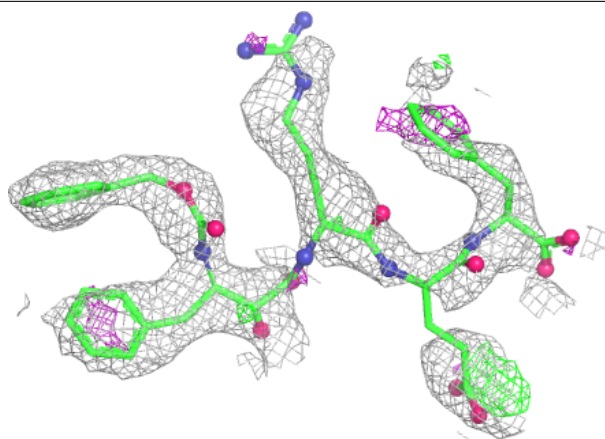
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DKT	C	1214	55/55	0.69	0.14	41,57,73,74	0
2	DKT	F	1214	55/55	0.70	0.14	41,57,73,74	0
2	DKT	E	1214	55/55	0.71	0.14	41,57,73,74	0
2	DKT	D	1214	55/55	0.75	0.12	41,57,73,74	0
2	DKT	B	1214	55/55	0.76	0.13	41,57,73,74	0
2	DKT	A	1214	55/55	0.78	0.13	41,57,73,74	0

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

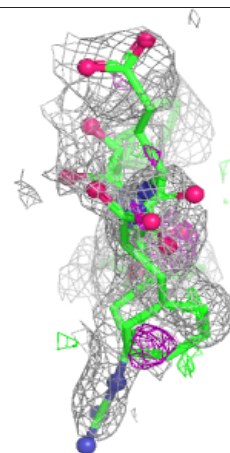
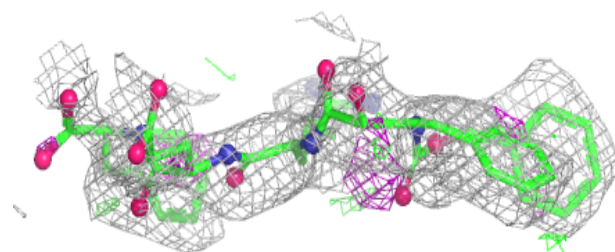
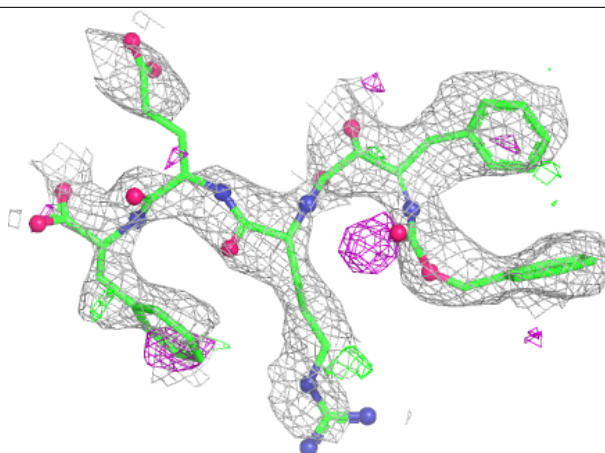
Electron density around DKT C 1214:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



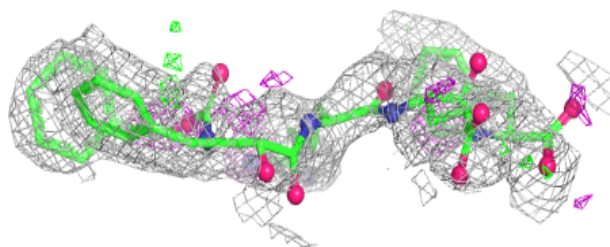
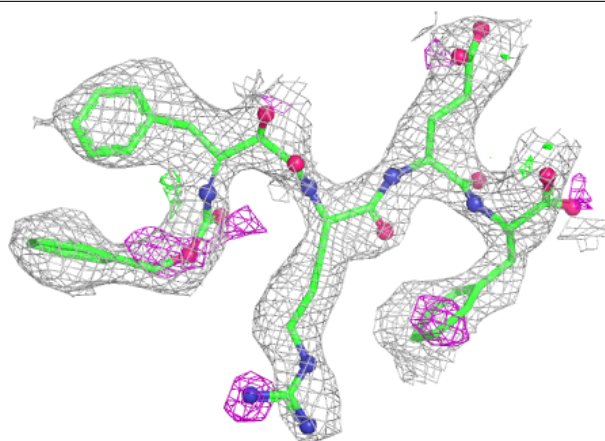
Electron density around DKT F 1214:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



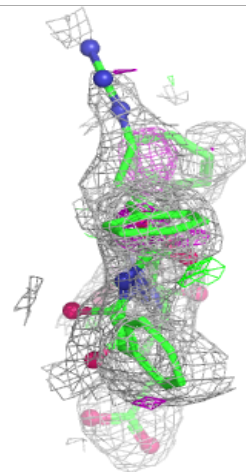
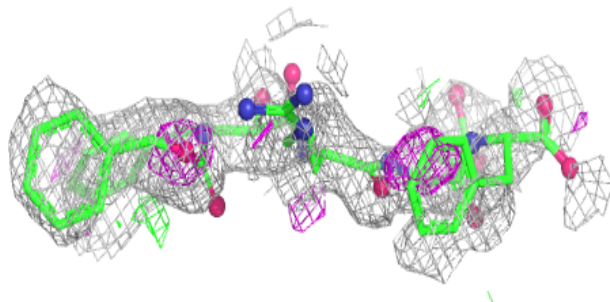
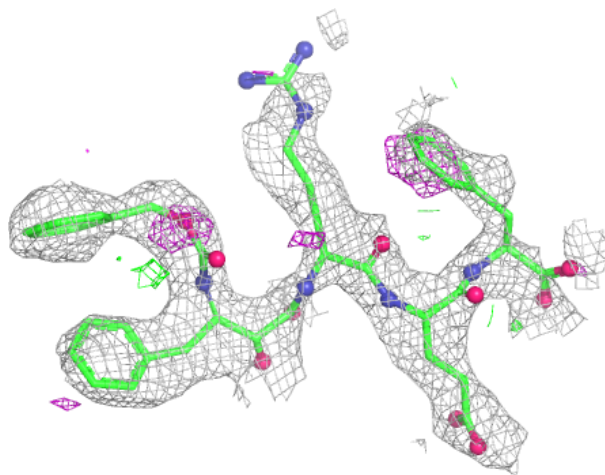
Electron density around DKT E 1214:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



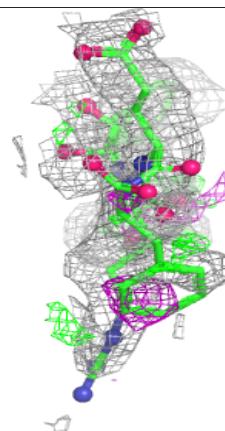
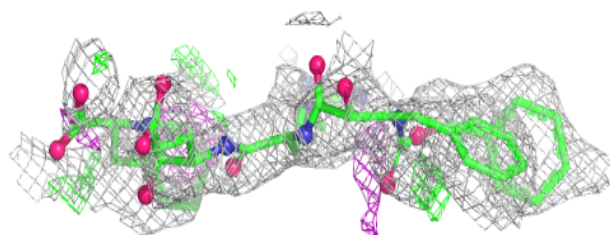
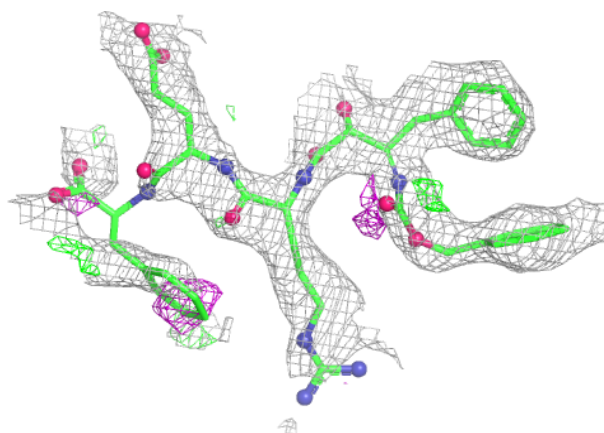
Electron density around DKT D 1214:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



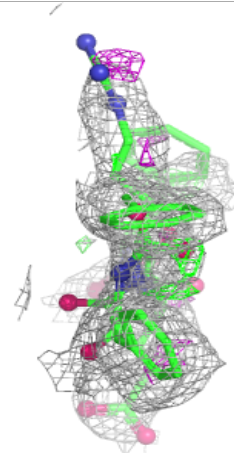
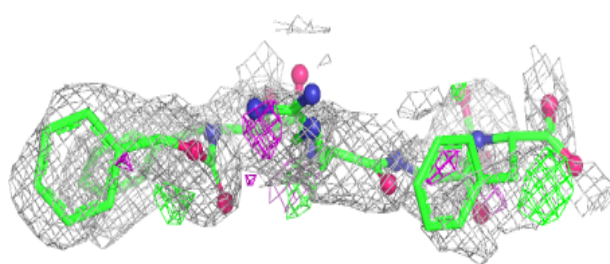
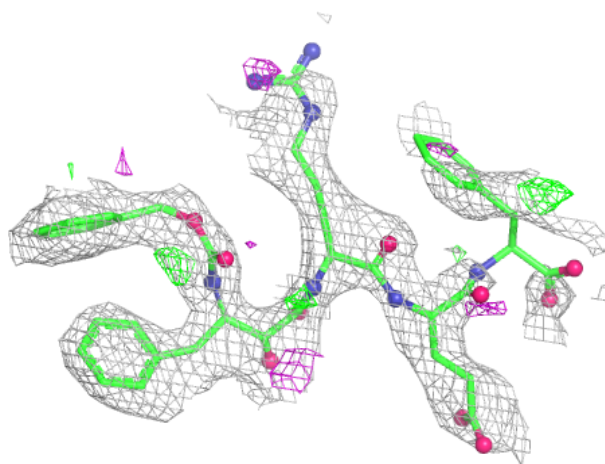
Electron density around DKT B 1214:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DKT A 1214:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.