



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 13, 2017 – 08:09 PM EDT

PDB ID : 5OG1  
EMDB ID: : EMD-3777  
Title : Cryo EM structure of the E. coli disaggregase ClpB (BAP form, DWB mutant),  
in the ATPgammaS state  
Authors : Deville, C.; Carroni, M.; Franke, K.B.; Topf, M.; Bukau, B.; Mogk, A.; Saibil,  
H.R.  
Deposited on : unknown  
Resolution : 4.50 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

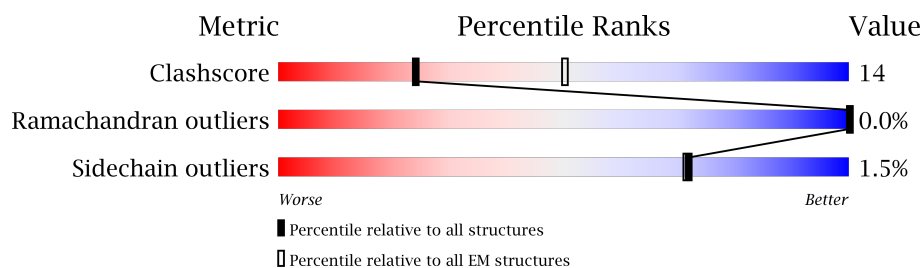
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	871	68% 25% 6%
1	B	871	45% 21% 34%
1	C	871	45% 26% 28%
1	D	871	49% 22% 28%
1	E	871	56% 22% 21%
1	F	871	53% 26% 21%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31380 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Chaperone protein ClpB,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	624	Total	C	N	O	S	0	0
			4960	3101	900	941	18		
1	F	686	Total	C	N	O	S	0	0
			5442	3401	985	1037	19		
1	E	686	Total	C	N	O	S	0	0
			5442	3401	985	1037	19		
1	D	624	Total	C	N	O	S	0	0
			4960	3101	900	941	18		
1	B	572	Total	C	N	O	S	0	0
			4518	2834	823	845	16		
1	A	819	Total	C	N	O	S	0	0
			5841	3667	1118	1037	19		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	MET	-	initiating methionine	UNP P63284
C	-2	ARG	-	expression tag	UNP P63284
C	-1	GLY	-	expression tag	UNP P63284
C	0	SER	-	expression tag	UNP P63284
C	279	ALA	GLU	engineered mutation	UNP P63284
C	678	ALA	GLU	engineered mutation	UNP P63284
C	745	ILE	ILE	linker	UNP P0ABH9
C	746	LYS	LYS	linker	UNP P0ABH9
C	747	LYS	LYS	linker	UNP P0ABH9
C	748	ILE	ILE	linker	UNP P0ABH9
C	858	GLY	-	expression tag	UNP P63284
C	859	SER	-	expression tag	UNP P63284
C	860	ARG	-	expression tag	UNP P63284
C	861	SER	-	expression tag	UNP P63284
C	862	HIS	-	expression tag	UNP P63284
C	863	HIS	-	expression tag	UNP P63284
C	864	HIS	-	expression tag	UNP P63284

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Chain	Residue	Modelled	Actual	Comment	Reference
C	865	HIS	-	expression tag	UNP P63284
C	866	HIS	-	expression tag	UNP P63284
C	867	HIS	-	expression tag	UNP P63284
F	-3	MET	-	initiating methionine	UNP P63284
F	-2	ARG	-	expression tag	UNP P63284
F	-1	GLY	-	expression tag	UNP P63284
F	0	SER	-	expression tag	UNP P63284
F	279	ALA	GLU	engineered mutation	UNP P63284
F	678	ALA	GLU	engineered mutation	UNP P63284
F	745	ILE	ILE	linker	UNP P0ABH9
F	746	LYS	LYS	linker	UNP P0ABH9
F	747	LYS	LYS	linker	UNP P0ABH9
F	748	ILE	ILE	linker	UNP P0ABH9
F	858	GLY	-	expression tag	UNP P63284
F	859	SER	-	expression tag	UNP P63284
F	860	ARG	-	expression tag	UNP P63284
F	861	SER	-	expression tag	UNP P63284
F	862	HIS	-	expression tag	UNP P63284
F	863	HIS	-	expression tag	UNP P63284
F	864	HIS	-	expression tag	UNP P63284
F	865	HIS	-	expression tag	UNP P63284
F	866	HIS	-	expression tag	UNP P63284
F	867	HIS	-	expression tag	UNP P63284
E	-3	MET	-	initiating methionine	UNP P63284
E	-2	ARG	-	expression tag	UNP P63284
E	-1	GLY	-	expression tag	UNP P63284
E	0	SER	-	expression tag	UNP P63284
E	279	ALA	GLU	engineered mutation	UNP P63284
E	678	ALA	GLU	engineered mutation	UNP P63284
E	745	ILE	ILE	linker	UNP P0ABH9
E	746	LYS	LYS	linker	UNP P0ABH9
E	747	LYS	LYS	linker	UNP P0ABH9
E	748	ILE	ILE	linker	UNP P0ABH9
E	858	GLY	-	expression tag	UNP P63284
E	859	SER	-	expression tag	UNP P63284
E	860	ARG	-	expression tag	UNP P63284
E	861	SER	-	expression tag	UNP P63284
E	862	HIS	-	expression tag	UNP P63284
E	863	HIS	-	expression tag	UNP P63284
E	864	HIS	-	expression tag	UNP P63284
E	865	HIS	-	expression tag	UNP P63284
E	866	HIS	-	expression tag	UNP P63284

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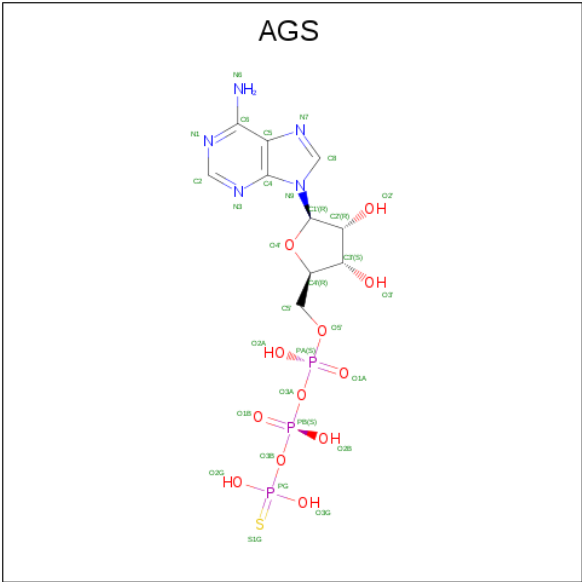
Chain	Residue	Modelled	Actual	Comment	Reference
E	867	HIS	-	expression tag	UNP P63284
D	-3	MET	-	initiating methionine	UNP P63284
D	-2	ARG	-	expression tag	UNP P63284
D	-1	GLY	-	expression tag	UNP P63284
D	0	SER	-	expression tag	UNP P63284
D	279	ALA	GLU	engineered mutation	UNP P63284
D	678	ALA	GLU	engineered mutation	UNP P63284
D	745	ILE	ILE	linker	UNP P0ABH9
D	746	LYS	LYS	linker	UNP P0ABH9
D	747	LYS	LYS	linker	UNP P0ABH9
D	748	ILE	ILE	linker	UNP P0ABH9
D	858	GLY	-	expression tag	UNP P63284
D	859	SER	-	expression tag	UNP P63284
D	860	ARG	-	expression tag	UNP P63284
D	861	SER	-	expression tag	UNP P63284
D	862	HIS	-	expression tag	UNP P63284
D	863	HIS	-	expression tag	UNP P63284
D	864	HIS	-	expression tag	UNP P63284
D	865	HIS	-	expression tag	UNP P63284
D	866	HIS	-	expression tag	UNP P63284
D	867	HIS	-	expression tag	UNP P63284
B	-3	MET	-	initiating methionine	UNP P63284
B	-2	ARG	-	expression tag	UNP P63284
B	-1	GLY	-	expression tag	UNP P63284
B	0	SER	-	expression tag	UNP P63284
B	279	ALA	GLU	engineered mutation	UNP P63284
B	678	ALA	GLU	engineered mutation	UNP P63284
B	745	ILE	ILE	linker	UNP P0ABH9
B	746	LYS	LYS	linker	UNP P0ABH9
B	747	LYS	LYS	linker	UNP P0ABH9
B	748	ILE	ILE	linker	UNP P0ABH9
B	858	GLY	-	expression tag	UNP P63284
B	859	SER	-	expression tag	UNP P63284
B	860	ARG	-	expression tag	UNP P63284
B	861	SER	-	expression tag	UNP P63284
B	862	HIS	-	expression tag	UNP P63284
B	863	HIS	-	expression tag	UNP P63284
B	864	HIS	-	expression tag	UNP P63284
B	865	HIS	-	expression tag	UNP P63284
B	866	HIS	-	expression tag	UNP P63284
B	867	HIS	-	expression tag	UNP P63284
A	-3	MET	-	initiating methionine	UNP P63284

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ARG	-	expression tag	UNP P63284
A	-1	GLY	-	expression tag	UNP P63284
A	0	SER	-	expression tag	UNP P63284
A	279	ALA	GLU	engineered mutation	UNP P63284
A	678	ALA	GLU	engineered mutation	UNP P63284
A	745	ILE	ILE	linker	UNP P0ABH9
A	746	LYS	LYS	linker	UNP P0ABH9
A	747	LYS	LYS	linker	UNP P0ABH9
A	748	ILE	ILE	linker	UNP P0ABH9
A	858	GLY	-	expression tag	UNP P63284
A	859	SER	-	expression tag	UNP P63284
A	860	ARG	-	expression tag	UNP P63284
A	861	SER	-	expression tag	UNP P63284
A	862	HIS	-	expression tag	UNP P63284
A	863	HIS	-	expression tag	UNP P63284
A	864	HIS	-	expression tag	UNP P63284
A	865	HIS	-	expression tag	UNP P63284
A	866	HIS	-	expression tag	UNP P63284
A	867	HIS	-	expression tag	UNP P63284

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						AltConf
2	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	

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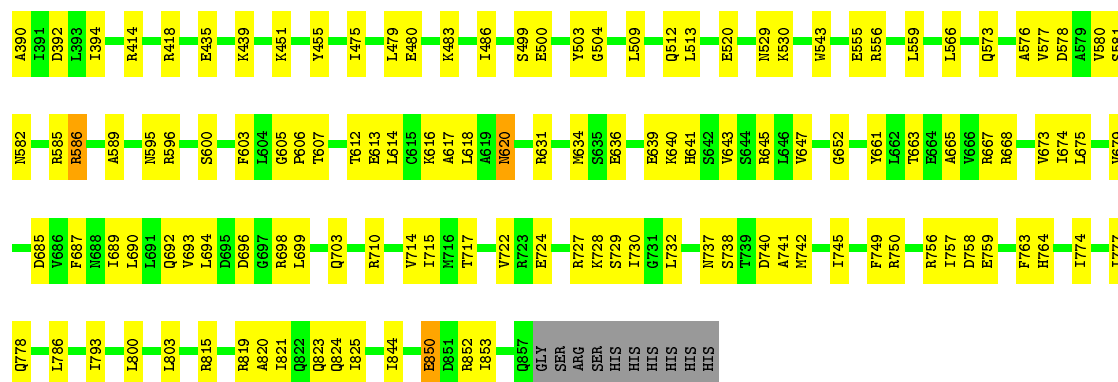
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Mol	Chain	Residues	Atoms						AltConf
2	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
2	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	



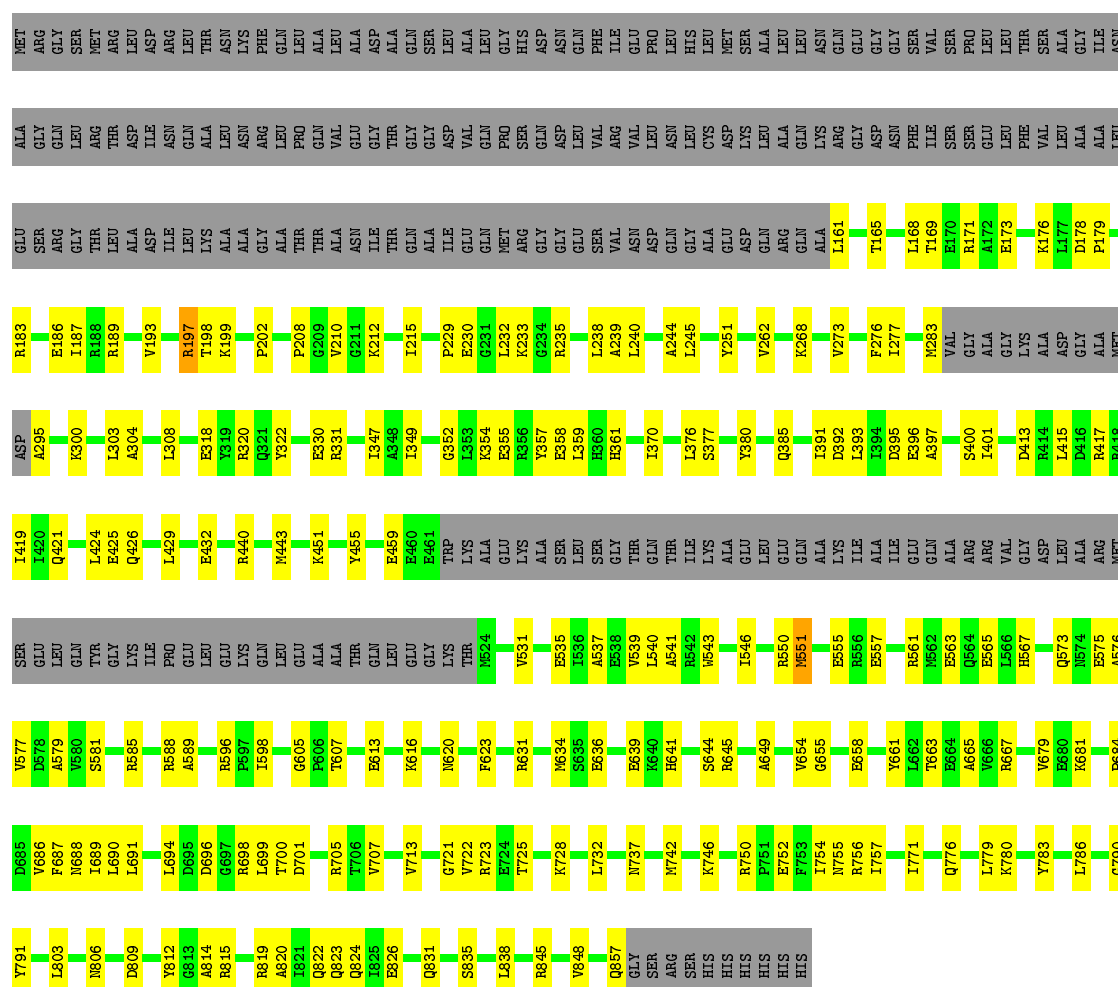






• Molecule 1: Chaperone protein ClpB,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB

Chain D: 49% 22% 28%



• Molecule 1: Chaperone protein ClpB,ATP-dependent Clp protease ATP-binding subunit ClpA,Chaperone protein ClpB

Chain B: 45% 21% 34%



6655	6656	6657	6658	6661	6662	6663	6664	6665	6666	6667	6672	6673	6674	6675	6676	6677	6686	6689	6690	6691	6692	6693	6699	6703	6704	6705	6713	6714	6715	6716	6717	6724	6725	6728	6729	6733	6734	6735	6738	6742	6750	6761	6762	6765	6766	6767	6768	6769	6770	6771	6772	6773	6774	6775	6776	6777	6778	6779	6783	6787	6793	6794	6795	6796	6797	6801	6802	6803	6807	6820	6821	6824	6825	6826	6827	6828	6829	6830	6831	6832	6833	6834	6835	6845	6846	6847	6848	6849	6854	6857	6858	6859	6860	6861	6862	6863	6864	6865	6866	6867	6868	6869	6870	6871	6872	6873	6874	6875	6876	6877	6878	6879	6880	6881	6882	6883	6884	6885	6886	6887	6888	6889	6890	6891	6892	6893	6894	6895	6896	6897	6898	6899	6900	6901	6902	6903	6904	6905	6906	6907	6908	6909	6910	6911	6912	6913	6914	6915	6916	6917	6918	6919	6920	6921	6922	6923	6924	6925	6926	6927	6928	6929	6930	6931	6932	6933	6934	6935	6936	6937	6938	6939	6940	6941	6942	6943	6944	6945	6946	6947	6948	6949	6950	6951	6952	6953	6954	6955	6956	6957	6958	6959	6960	6961	6962	6963	6964	6965	6966	6967	6968	6969	6970	6971	6972	6973	6974	6975	6976	6977	6978	6979	6980	6981	6982	6983	6984	6985	6986	6987	6988	6989	6990	6991	6992	6993	6994	6995	6996	6997	6998	6999	7000	7001	7002	7003	7004	7005	7006	7007	7008	7009	7010	7011	7012	7013	7014	7015	7016	7017	7018	7019	7020	7021	7022	7023	7024	7025	7026	7027	7028	7029	7030	7031	7032	7033	7034	7035	7036	7037	7038	7039	7040	7041	7042	7043	7044	7045	7046	7047	7048	7049	7050	7051	7052	7053	7054	7055	7056	7057	7058	7059	7060	7061	7062	7063	7064	7065	7066	7067	7068	7069	7070	7071	7072	7073	7074	7075	7076	7077	7078	7079	7080	7081	7082	7083	7084	7085	7086	7087	7088	7089	7090	7091	7092	7093	7094	7095	7096	7097	7098	7099	7100	7101	7102	7103	7104	7105	7106	7107	7108	7109	7110	7111	7112	7113	7114	7115	7116	7117	7118	7119	7120	7121	7122	7123	7124	7125	7126	7127	7128	7129	7130	7131	7132	7133	7134	7135	7136	7137	7138	7139	7140	7141	7142	7143	7144	7145	7146	7147	7148	7149	7150	7151	7152	7153	7154	7155	7156	7157	7158	7159	7160	7161	7162	7163	7164	7165	7166	7167	7168	7169	7170	7171	7172	7173	7174	7175	7176	7177	7178	7179	7180	7181	7182	7183	7184	7185	7186	7187	7188	7189	7190	7191	7192	7193	7194	7195	7196	7197	7198	7199	7200	7201	7202	7203	7204	7205	7206	7207	7208	7209	7210	7211	7212	7213	7214	7215	7216	7217	7218	7219	7220	7221	7222	7223	7224	7225	7226	7227	7228	7229	7230	7231	7232	7233	7234	7235	7236	7237	7238	7239	7240	7241	7242	7243	7244	7245	7246	7247	7248	7249	7250	7251	7252	7253	7254	7255	7256	7257	7258	7259	7260	7261	7262	7263	7264	7265	7266	7267	7268	7269	7270	7271	7272	7273	7274	7275	7276	7277	7278	7279	7280	7281	7282	7283	7284	7285	7286	7287	7288	7289	7290	7291	7292	7293	7294	7295	7296	7297	7298	7299	7300	7301	7302	7303	7304	7305	7306	7307	7308	7309	7310	7311	7312	7313	7314	7315	7316	7317	7318	7319	7320	7321	7322	7323	7324	7325	7326	7327	7328	7329	7330	7331	7332	7333	7334	7335	7336	7337	7338	7339	7340	7341	7342	7343	7344	7345	7346	7347	7348	7349	7350	7351	7352	7353	7354	7355	7356	7357	7358	7359	7360	7361	7362	7363	7364	7365	7366	7367	7368	7369	7370	7371	7372	7373	7374	7375	7376	7377	7378	7379	7380	7381	7382	7383	7384	7385	7386	7387	7388	7389	7390	7391	7392	7393	7394	7395	7396	7397	7398	7399	7400	7401	7402	7403	7404	7405	7406	7407	7408	7409	7410	7411	7412	7413	7414	7415	7416	7417	7418	7419	7420	7421	7422	7423	7424	7425	7426	7427	7428	7429	7430	7431	7432	7433	7434	7435	7436	7437	7438	7439	7440	7441	7442	7443	7444	7445	7446	7447	7448	7449	7450	7451	7452	7453	7454	7455	7456	7457	7458	7459	7460	7461	7462	7463	7464	7465	7466	7467	7468	7469	7470	7471	7472	7473	7474	7475	7476	7477	7478	7479	7480	7481	7482	7483	7484	7485	7486	7487	7488	7489	7490	7491	7492	7493	7494	7495	7496	7497	7498	7499	7500	7501	7502	7503	7504	7505	7506	7507	7508	7509	7510	7511	7512	7513	7514	7515	7516	7517	7518	7519	7520	7521	7522	7523	7524	7525	7526	7527	7528	7529	7530	7531	7532	7533	7534	7535	7536	7537	7538	7539	7540	7541	7542	7543	7544	7545	7546	7547	7548	7549	7550	7551	7552	7553	7554	7555	7556	7557	7558	7559	7560	7561	7562	7563	7564	7565	7566	7567	7568	7569	7570	7571	7572	7573	7574	7575	7576	7577	7578	7579	7580	7581	7582	7583	7584	7585	7586	7587	7588	7589	7590	7591	7592	7593	7594	7595	7596	7597	7598	7599	7600	7601	7602	7603	7604	7605	7606	7607	7608	7609	7610	7611	7612	7613	7614	7615	7616	7617	7618	7619	7620	7621	7622	7623	7624	7625	7626	7627	7628	7629	7630	7631	7632	7633	7634	7635	7636	7637	7638	7639	7640	7641	7642	7643	7644	7645	7646	7647	7648	7649	7650	7651	7652	7653	7654	7655	7656	7657	7658	7659	7660	7661	7662	7663	7664	7665	7666	7667	7668	7669	7670	7671	7672	7673	7674	7675	7676	7677	7678	7679	7680	7681	7682	7683	7684	7685	7686	7687	7688	7689	7690	7691	7692	7693	7694	7695	7696	7697	7698	7699	7700	7701	7702	7703	7704	7705	7706	7707	7708	7709	7710	7711	7712	7713	7714	7715	7716	7717	7718	7719	7720	7721	7722	7723	7724	7725	7726	7727	7728	7729	7730	7731	7732	7733	7734	7735	7736	7737	7738	7739	7740	7741	7742	7743	7744	7745	7746	7747	7748	7749	7750	7751	7752	7753	7754	7755	7756	7757	7758	7759	7760	7761	7762	7763	7764	7765	7766	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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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  >2	RMSZ	# Z  >2
1	A	0.31	0/5909	0.60	2/7815 (0.0%)
1	B	0.33	0/4582	0.64	3/6178 (0.0%)
1	C	0.34	0/5025	0.64	0/6766
1	D	0.32	0/5025	0.62	0/6766
1	E	0.31	0/5512	0.60	1/7420 (0.0%)
1	F	0.32	0/5512	0.61	1/7420 (0.0%)
All	All	0.32	0/31565	0.62	7/42365 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	0	3
1	C	0	1
1	D	0	4
1	E	0	1
1	F	0	2
All	All	1	11

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	682	ALA	C-N-CA	6.61	138.21	121.70
1	E	194	LEU	CA-CB-CG	6.37	129.96	115.30
1	B	194	LEU	CA-CB-CG	6.37	129.95	115.30
1	B	691	LEU	CB-CG-CD2	-5.65	101.39	111.00

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	GLY	N-CA-C	5.59	127.07	113.10
1	F	339	ALA	C-N-CA	5.27	134.87	121.70
1	A	271	GLY	C-N-CA	5.16	134.61	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	72	PRO	CA

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	198	THR	Peptide
1	B	322	TYR	Peptide
1	B	405	ILE	Peptide
1	C	409	PRO	Peptide
1	D	550	ARG	Peptide
1	D	551	MET	Peptide
1	D	623	PHE	Peptide
1	D	848	VAL	Peptide
1	E	850	GLU	Peptide
1	F	636	GLU	Peptide
1	F	638	MET	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5841	0	5696	169	0
1	B	4518	0	4613	121	0
1	C	4960	0	5051	177	0
1	D	4960	0	5051	140	0
1	E	5442	0	5552	144	0
1	F	5442	0	5551	176	0
2	B	31	0	12	4	0
2	C	62	0	24	4	0
2	D	62	0	24	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	62	0	24	10	0
All	All	31380	0	31598	858	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 14.

All (858) 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:E:251:TYR:CE1	1:A:73:GLN:N	2.07	1.22
1:E:614:LEU:O	1:E:618:LEU:HB2	1.54	1.06
1:B:663:THR:O	1:B:667:ARG:HB2	1.59	1.03
1:F:663:THR:O	1:F:667:ARG:HB2	1.57	1.01
1:C:357:TYR:O	1:C:361:HIS:HB2	1.58	1.01
1:C:643:VAL:O	1:C:647:VAL:HB	1.61	1.00
1:E:318:GLU:O	1:E:322:TYR:HB2	1.62	1.00
1:C:743:GLU:O	1:C:747:LYS:HB2	1.63	0.99
1:D:820:ALA:O	1:D:824:GLN:HB2	1.63	0.98
1:D:251:TYR:CZ	1:A:74:VAL:CA	2.48	0.96
1:E:577:VAL:O	1:E:581:SER:HB2	1.66	0.95
1:C:617:ALA:O	1:C:621:PHE:HB2	1.66	0.95
1:C:663:THR:O	1:C:667:ARG:HB2	1.68	0.94
1:F:820:ALA:O	1:F:824:GLN:HB2	1.66	0.94
1:A:500:GLU:O	1:A:504:GLY:HA3	1.66	0.94
1:A:783:TYR:O	1:A:787:GLU:HB2	1.69	0.93
1:E:251:TYR:HE1	1:A:73:GLN:N	1.49	0.93
1:D:819:ARG:O	1:D:823:GLN:HB3	1.67	0.92
1:B:783:TYR:O	1:B:787:GLU:HB2	1.71	0.90
1:E:500:GLU:O	1:E:504:GLY:HA3	1.70	0.90
1:D:251:TYR:CE1	1:A:74:VAL:CA	2.55	0.90
1:D:251:TYR:CE1	1:A:74:VAL:C	2.46	0.88
1:E:251:TYR:HE1	1:A:73:GLN:CA	1.86	0.87
1:E:357:TYR:O	1:E:361:HIS:HB2	1.75	0.86
1:A:355:GLU:O	1:A:359:LEU:HB2	1.76	0.86
1:B:821:ILE:O	1:B:825:ILE:HB	1.75	0.86
1:E:251:TYR:CZ	1:A:73:GLN:N	2.43	0.85
1:D:391:ILE:O	1:D:395:ASP:HB2	1.77	0.84
1:B:373:ALA:O	1:B:377:SER:HB3	1.75	0.84
1:F:221:GLN:O	1:F:225:ASN:HB2	1.76	0.84
1:E:373:ALA:O	1:E:377:SER:HB3	1.78	0.84
1:F:576:ALA:O	1:F:580:VAL:HB	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:475:ILE:O	1:E:479:LEU:HB2	1.80	0.81
1:D:686:VAL:O	1:D:690:LEU:HB2	1.80	0.81
1:A:724:GLU:O	1:A:728:LYS:HB3	1.79	0.81
1:D:419:ILE:HG22	1:D:451:LYS:HB3	1.62	0.81
1:E:578:ASP:O	1:E:582:ASN:HB2	1.81	0.81
1:A:643:VAL:O	1:A:647:VAL:HB	1.82	0.80
1:A:821:ILE:O	1:A:825:ILE:HB	1.82	0.80
1:F:251:TYR:HE1	1:A:69:ASN:CA	1.94	0.79
1:D:357:TYR:O	1:D:361:HIS:HB2	1.82	0.79
1:F:469:LEU:O	1:F:473:GLN:HB2	1.85	0.77
1:F:169:THR:O	1:F:173:GLU:HB2	1.85	0.77
1:F:830:ALA:O	1:F:834:LEU:HB2	1.84	0.77
1:A:738:SER:O	1:A:742:MET:HB2	1.85	0.77
1:E:616:LYS:O	1:E:620:ASN:HB2	1.85	0.77
1:F:802:LEU:O	1:F:806:ASN:HB2	1.84	0.76
1:E:663:THR:O	1:E:667:ARG:HB2	1.85	0.76
1:F:686:VAL:O	1:F:690:LEU:HB3	1.85	0.76
1:D:819:ARG:HG2	1:D:822:GLN:HE21	1.52	0.75
1:C:576:ALA:O	1:C:580:VAL:HB	1.86	0.75
1:C:578:ASP:O	1:C:582:ASN:HB2	1.86	0.75
1:E:738:SER:O	1:E:742:MET:HB2	1.86	0.74
1:A:402:ARG:O	1:A:406:ASP:HB2	1.88	0.74
1:E:251:TYR:CE1	1:A:73:GLN:CA	2.67	0.73
1:F:509:LEU:O	1:F:513:LEU:HB2	1.89	0.73
1:E:323:ILE:HG13	1:E:325:LYS:H	1.54	0.72
1:A:752:GLU:HA	1:A:755:ASN:HB2	1.73	0.71
1:C:372:ALA:O	1:C:376:LEU:HB2	1.91	0.70
1:B:583:ALA:O	1:B:587:SER:HB3	1.91	0.70
1:F:687:PHE:O	1:F:691:LEU:HB2	1.92	0.70
1:B:221:GLN:O	1:B:225:ASN:HB2	1.91	0.69
1:C:783:TYR:O	1:C:787:GLU:HB2	1.91	0.69
1:D:663:THR:O	1:D:667:ARG:HB2	1.93	0.69
1:B:800:LEU:O	1:B:804:SER:HB3	1.94	0.68
1:D:631:ARG:NH2	2:D:902:AGS:O2G	2.27	0.68
1:F:797:ASP:O	1:F:801:LYS:HB2	1.94	0.68
1:A:412:LEU:O	1:A:416:ASP:HB2	1.95	0.67
1:C:619:ALA:O	1:C:623:PHE:HB2	1.93	0.67
1:D:585:ARG:O	1:D:589:ALA:HB2	1.94	0.67
1:C:821:ILE:O	1:C:825:ILE:HB	1.94	0.67
1:A:655:GLY:HA2	1:A:658:GLU:HB3	1.77	0.67
1:C:451:LYS:O	1:C:455:TYR:HB3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:577:VAL:O	1:C:581:SER:HB2	1.94	0.67
1:F:277:ILE:HD13	1:F:283:MET:HG3	1.76	0.67
1:C:429:LEU:O	1:C:439:LYS:NZ	2.28	0.67
1:C:457:GLU:O	1:C:461:GLU:HB3	1.95	0.67
1:A:222:ARG:HG3	1:A:227:GLU:HB2	1.75	0.66
1:C:618:LEU:HD23	1:C:715:ILE:HD11	1.76	0.66
1:E:674:ILE:HB	1:E:714:VAL:HA	1.78	0.66
1:C:373:ALA:O	1:C:377:SER:HB3	1.95	0.65
1:A:444:LEU:O	1:A:448:LEU:HB2	1.96	0.65
1:D:212:LYS:HA	1:D:215:ILE:HD12	1.78	0.65
1:E:821:ILE:O	1:E:825:ILE:HB	1.96	0.65
1:B:380:TYR:OH	1:B:711:ASN:ND2	2.30	0.65
1:D:318:GLU:O	1:D:322:TYR:HB2	1.97	0.65
1:E:435:GLU:O	1:E:439:LYS:HB2	1.96	0.65
1:C:170:GLU:HG2	1:C:174:GLN:HE22	1.62	0.65
1:E:499:SER:O	1:E:503:TYR:HB2	1.96	0.65
1:B:375:THR:O	1:B:379:ARG:HB2	1.96	0.64
1:F:164:TYR:OH	1:F:258:ARG:NH1	2.30	0.64
1:E:603:PHE:HB2	1:E:717:THR:HA	1.78	0.64
1:C:577:VAL:O	1:C:581:SER:CB	2.46	0.64
1:A:242:MET:SD	1:A:282:THR:OG1	2.55	0.64
1:C:674:ILE:HB	1:C:714:VAL:HG23	1.79	0.64
1:E:631:ARG:HD3	1:D:698:ARG:HD2	1.80	0.64
1:C:318:GLU:O	1:C:322:TYR:HB2	1.98	0.64
1:E:509:LEU:O	1:E:513:LEU:HB2	1.98	0.64
1:A:204:LEU:HB3	1:A:212:LYS:HD2	1.81	0.63
1:B:350:LEU:HD22	1:B:394:ILE:HD12	1.80	0.63
1:F:475:ILE:O	1:F:479:LEU:HB2	1.98	0.63
1:C:750:ARG:HG2	1:D:722:VAL:HG21	1.81	0.63
1:E:197:ARG:O	1:E:332:ARG:NH1	2.32	0.63
1:F:196:ARG:HE	1:A:396:GLU:HB2	1.62	0.63
1:D:239:ALA:HA	1:D:276:PHE:HB3	1.80	0.63
1:E:170:GLU:HG2	1:E:174:GLN:HE22	1.62	0.63
1:F:605:GLY:O	1:F:719:ASN:ND2	2.32	0.63
1:F:161:LEU:N	1:F:265:ASP:OD2	2.32	0.63
1:E:184:ASP:OD1	1:E:222:ARG:NH2	2.31	0.63
1:D:169:THR:O	1:D:173:GLU:HB2	1.98	0.62
1:E:774:ILE:O	1:E:778:GLN:HB2	1.98	0.62
1:F:559:LEU:HB3	1:F:585:ARG:HG2	1.81	0.62
1:D:742:MET:O	1:D:746:LYS:HB2	1.99	0.62
1:E:737:ASN:O	1:E:741:ALA:HB3	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:662:LEU:O	1:F:666:VAL:HB	2.00	0.62
1:C:327:ALA:HA	1:C:330:GLU:HG2	1.82	0.62
1:C:690:LEU:O	1:C:694:LEU:HB2	1.99	0.62
1:D:831:GLN:O	1:D:835:SER:HB2	1.99	0.62
1:F:391:ILE:O	1:F:395:ASP:HB2	2.00	0.62
1:F:263:LEU:O	1:F:267:ALA:HB2	2.00	0.61
1:F:469:LEU:HD11	1:F:529:ASN:HD21	1.65	0.61
1:B:669:ARG:NE	1:B:671:TYR:O	2.34	0.61
1:C:457:GLU:O	1:C:461:GLU:CB	2.49	0.61
1:E:696:ASP:O	1:E:698:ARG:NH1	2.34	0.61
1:D:531:VAL:HA	1:D:535:GLU:HG3	1.82	0.61
1:A:769:GLN:O	1:A:773:SER:HB2	1.99	0.61
1:B:240:LEU:H	1:B:275:LEU:HD11	1.66	0.61
1:B:831:GLN:O	1:B:835:SER:HB2	2.00	0.61
1:D:691:LEU:HD22	1:D:750:ARG:HH21	1.65	0.61
1:D:644:SER:HB3	1:D:649:ALA:HA	1.82	0.61
1:F:356:ARG:O	1:F:360:HIS:HB3	2.01	0.61
1:A:663:THR:O	1:A:667:ARG:HB2	2.00	0.61
1:C:537:ALA:O	1:C:541:ALA:HB2	2.01	0.61
1:A:617:ALA:O	1:A:621:PHE:HB2	2.01	0.61
1:A:794:HIS:HB2	1:A:845:ARG:HG2	1.82	0.61
1:E:366:THR:HG22	1:E:368:PRO:HD2	1.83	0.61
1:F:297:ASN:HB3	1:A:246:VAL:HG21	1.82	0.60
1:C:781:ARG:HG2	1:C:785:ARG:HE	1.66	0.60
1:B:276:PHE:HA	1:B:311:VAL:HB	1.82	0.60
1:E:183:ARG:HH12	1:E:341:PRO:HB3	1.66	0.60
1:F:819:ARG:O	1:F:823:GLN:HB3	2.02	0.60
1:F:577:VAL:O	1:F:581:SER:HB2	2.01	0.60
1:B:315:THR:O	1:B:319:TYR:N	2.33	0.60
1:B:698:ARG:HA	1:B:709:PHE:H	1.66	0.60
1:A:674:ILE:HB	1:A:714:VAL:HA	1.83	0.60
1:C:831:GLN:O	1:C:835:SER:HB2	2.01	0.60
1:E:645:ARG:NH2	1:D:701:ASP:O	2.35	0.60
1:B:223:ILE:HG12	1:B:232:LEU:HB3	1.84	0.60
1:C:759:GLU:OE2	1:D:823:GLN:NE2	2.35	0.60
1:D:655:GLY:HA2	1:D:658:GLU:HB2	1.83	0.60
1:D:197:ARG:NH1	1:D:198:THR:OG1	2.35	0.60
1:C:208:PRO:HB2	1:B:327:ALA:HB3	1.83	0.59
1:A:280:LEU:HD22	1:A:312:GLY:HA3	1.84	0.59
1:A:703:GLN:HG2	1:A:705:ARG:HH21	1.68	0.59
1:E:605:GLY:HA3	1:E:763:PHE:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:PRO:HG2	1:F:311:VAL:HG13	1.84	0.59
1:A:661:TYR:O	1:A:665:ALA:HB2	2.03	0.59
1:D:421:GLN:O	1:D:425:GLU:HB2	2.02	0.59
1:E:698:ARG:HD2	1:E:710:ARG:HH11	1.67	0.59
1:B:399:SER:HA	1:B:402:ARG:HE	1.68	0.59
1:D:413:ASP:O	1:D:417:ARG:HB2	2.02	0.59
1:C:722:VAL:O	1:C:726:GLU:HB2	2.02	0.59
1:F:400:SER:OG	1:E:195:GLN:NE2	2.36	0.59
1:A:596:ARG:NH2	1:A:756:ARG:O	2.36	0.59
1:A:649:ALA:HB1	1:A:653:TYR:HB3	1.84	0.59
1:F:786:LEU:HB3	1:F:791:TYR:HB2	1.85	0.59
1:C:541:ALA:HB1	1:C:547:PRO:HA	1.84	0.59
1:D:551:MET:O	1:D:555:GLU:HB2	2.02	0.59
1:A:509:LEU:O	1:A:513:LEU:HB2	2.02	0.58
1:E:673:VAL:HG13	1:E:715:ILE:HD12	1.84	0.58
2:E:901:AGS:O1B	2:E:901:AGS:S1G	2.61	0.58
1:C:636:GLU:O	1:C:645:ARG:NH1	2.36	0.58
1:D:183:ARG:NH1	1:D:186:GLU:OE2	2.30	0.58
1:F:726:GLU:HG2	1:F:765:PRO:HG2	1.85	0.58
1:D:809:ASP:HB3	1:D:812:TYR:HB2	1.84	0.58
1:E:727:ARG:NH2	1:E:740:ASP:OD2	2.36	0.58
1:A:631:ARG:HG2	1:A:675:LEU:HD23	1.84	0.58
1:F:318:GLU:O	1:F:322:TYR:HB2	2.03	0.58
1:C:181:ILE:HG23	1:D:424:LEU:HB3	1.85	0.58
1:C:426:GLN:HA	1:C:429:LEU:HB2	1.86	0.58
1:F:377:SER:HB2	1:F:389:LYS:HD2	1.84	0.58
1:F:573:GLN:HB3	1:F:576:ALA:HB3	1.85	0.58
1:F:169:THR:O	1:F:173:GLU:CB	2.51	0.58
1:F:469:LEU:HA	1:F:472:THR:HG22	1.85	0.58
1:A:314:THR:OG1	1:A:318:GLU:OE1	2.22	0.58
1:B:242:MET:HA	1:B:245:LEU:HD12	1.86	0.58
1:C:357:TYR:HA	1:C:360:HIS:HB3	1.85	0.58
1:E:639:GLU:OE2	1:E:645:ARG:NH1	2.34	0.58
1:E:573:GLN:NE2	1:E:764:HIS:O	2.35	0.58
1:E:820:ALA:HA	1:E:823:GLN:HG2	1.86	0.58
1:A:242:MET:HA	1:A:245:LEU:HB2	1.86	0.57
1:A:329:LEU:O	1:A:333:PHE:N	2.37	0.57
1:D:187:ILE:HG12	1:D:215:ILE:HG23	1.84	0.57
1:A:676:LEU:HB2	1:A:716:MET:HA	1.86	0.57
1:C:826:GLU:HB3	1:B:591:LEU:HD23	1.86	0.57
1:D:561:ARG:NH1	1:D:565:GLU:OE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:314:THR:OG1	1:E:318:GLU:OE1	2.22	0.57
1:F:196:ARG:NH2	1:A:396:GLU:OE1	2.38	0.57
1:E:631:ARG:NH2	2:E:902:AGS:O3G	2.38	0.57
1:A:359:LEU:HD21	1:A:479:LEU:HD12	1.87	0.57
1:E:211:GLY:O	1:E:215:ILE:N	2.37	0.57
1:F:509:LEU:HD23	1:F:512:GLN:HE21	1.69	0.57
1:F:537:ALA:O	1:F:541:ALA:CB	2.53	0.57
1:A:657:GLU:HA	1:A:703:GLN:HE22	1.70	0.57
1:F:577:VAL:O	1:F:581:SER:CB	2.53	0.57
1:F:596:ARG:HH22	1:F:756:ARG:HB3	1.70	0.57
1:F:388:ASP:OD2	1:E:331:ARG:NH1	2.38	0.57
1:F:344:GLU:HA	1:F:347:ILE:HD12	1.86	0.56
1:F:803:LEU:HD22	1:F:821:ILE:HA	1.86	0.56
1:D:168:LEU:HD23	1:D:171:ARG:HD3	1.87	0.56
1:D:393:LEU:O	1:D:397:ALA:CB	2.54	0.56
1:E:237:VAL:HG22	1:E:274:ILE:HB	1.87	0.56
1:F:374:ALA:O	1:F:378:HIS:HB2	2.06	0.56
1:C:745:ILE:O	1:C:749:PHE:N	2.37	0.56
1:B:222:ARG:HG2	1:B:228:VAL:HB	1.87	0.56
1:D:684:PRO:O	1:D:688:ASN:ND2	2.38	0.56
1:E:354:LYS:HB2	1:E:365:ILE:HG13	1.87	0.56
1:F:405:ILE:HA	1:F:527:LEU:HD22	1.88	0.56
1:A:174:GLN:HG2	1:A:176:LYS:HE2	1.87	0.56
1:C:579:ALA:HB1	1:C:759:GLU:HG3	1.87	0.56
1:F:222:ARG:O	1:F:227:GLU:N	2.39	0.56
1:F:778:GLN:HE21	1:F:818:LYS:HD3	1.71	0.56
1:C:678:ALA:H	1:C:718:SER:HA	1.71	0.56
1:F:686:VAL:O	1:F:690:LEU:CB	2.53	0.56
1:B:240:LEU:HD22	1:B:262:VAL:HG11	1.87	0.56
1:B:663:THR:HA	1:B:666:VAL:HG22	1.88	0.56
1:E:640:LYS:NZ	1:E:685:ASP:OD2	2.39	0.56
1:F:596:ARG:HH12	1:F:756:ARG:HD3	1.71	0.56
1:A:803:LEU:HD11	1:A:825:ILE:HD11	1.86	0.56
1:C:222:ARG:HG3	1:C:227:GLU:HB2	1.88	0.56
1:A:573:GLN:HB3	1:A:576:ALA:HB3	1.86	0.55
1:C:724:GLU:O	1:C:728:LYS:HB3	2.07	0.55
1:E:643:VAL:O	1:E:647:VAL:HB	2.06	0.55
1:A:827:ASN:O	1:A:831:GLN:HB2	2.06	0.55
1:F:396:GLU:HB2	1:E:196:ARG:HE	1.71	0.55
1:F:394:ILE:O	1:F:398:ALA:CB	2.53	0.55
1:F:550:ARG:NE	1:F:624:ASP:OD1	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ALA:O	1:A:258:ARG:NH1	2.40	0.55
1:A:630:VAL:HB	1:A:674:ILE:HA	1.89	0.55
1:D:819:ARG:O	1:D:823:GLN:CB	2.50	0.55
1:A:250:LYS:HB2	1:A:254:GLU:HG3	1.88	0.55
1:C:616:LYS:O	1:C:620:ASN:HB2	2.06	0.55
1:F:170:GLU:HA	1:F:173:GLU:HB3	1.88	0.55
1:F:326:ASP:HB3	1:F:329:LEU:HB2	1.88	0.55
1:F:780:LYS:HA	1:F:783:TYR:HD2	1.72	0.55
1:F:619:ALA:O	1:F:623:PHE:HB2	2.07	0.55
1:C:758:ASP:HA	1:D:819:ARG:HH21	1.71	0.55
1:A:369:ALA:O	1:A:373:ALA:HB2	2.07	0.55
1:C:410:GLU:H	1:C:526:LEU:HD22	1.71	0.55
2:C:901:AGS:O3B	2:C:901:AGS:O2A	2.25	0.55
1:C:267:ALA:HA	1:C:307:GLU:HB3	1.89	0.55
1:D:303:LEU:HD23	1:D:308:LEU:HD21	1.88	0.55
1:D:699:LEU:HB3	1:D:707:VAL:HB	1.87	0.55
1:F:825:ILE:O	1:F:829:LEU:N	2.37	0.55
1:B:376:LEU:HA	1:B:379:ARG:HB3	1.89	0.55
1:C:373:ALA:O	1:C:377:SER:CB	2.55	0.55
1:F:189:ARG:NH1	1:A:396:GLU:OE2	2.39	0.54
1:B:166:ILE:HG21	1:A:305:ARG:HD2	1.89	0.54
1:E:634:MET:HG3	1:E:679:VAL:HG23	1.88	0.54
1:B:269:GLN:HG2	1:B:272:ASN:HB2	1.87	0.54
1:C:199:LYS:HB3	1:C:334:GLN:HB2	1.90	0.54
1:C:409:PRO:HB2	1:C:412:LEU:HD13	1.88	0.54
1:C:458:LEU:HA	1:C:461:GLU:HB3	1.88	0.54
1:C:583:ALA:O	1:C:587:SER:HB3	2.08	0.54
1:F:496:ALA:O	1:F:500:GLU:HB2	2.07	0.54
1:A:300:LYS:O	1:A:304:ALA:HB2	2.07	0.54
1:A:520:GLU:HG2	1:A:524:MET:HG3	1.89	0.54
1:C:632:ILE:HD11	1:C:665:ALA:HB3	1.88	0.54
1:D:393:LEU:O	1:D:397:ALA:HB2	2.06	0.54
1:E:692:GLN:O	1:E:696:ASP:HB2	2.06	0.54
1:E:595:ASN:OD1	1:E:698:ARG:NH1	2.40	0.54
1:F:602:LEU:HD22	1:F:753:PHE:HE2	1.72	0.54
1:A:393:LEU:HD11	1:A:540:LEU:HD13	1.87	0.54
1:C:350:LEU:HB3	1:C:370:ILE:HB	1.89	0.54
1:E:786:LEU:HD13	1:E:793:ILE:HD12	1.88	0.54
1:F:183:ARG:HD3	1:F:215:ILE:HG12	1.90	0.54
1:B:181:ILE:HD13	1:B:349:ILE:HA	1.89	0.54
1:B:361:HIS:HA	1:B:402:ARG:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:TYR:O	1:D:459:GLU:HB2	2.08	0.54
1:F:831:GLN:O	1:F:835:SER:CB	2.55	0.54
1:F:591:LEU:HD21	1:A:830:ALA:HB3	1.89	0.54
1:A:796:SER:OG	1:A:845:ARG:NH2	2.41	0.54
1:B:536:ILE:O	1:B:540:LEU:HB3	2.08	0.54
1:F:638:MET:N	1:F:638:MET:SD	2.79	0.54
1:A:604:LEU:HB2	1:A:762:VAL:HG22	1.89	0.53
1:B:328:ALA:O	1:B:331:ARG:N	2.40	0.53
1:E:728:LYS:HD3	1:E:737:ASN:HD22	1.72	0.53
1:F:373:ALA:O	1:F:377:SER:OG	2.22	0.53
1:B:588:ARG:HA	1:B:598:ILE:HD13	1.89	0.53
1:C:349:ILE:HG13	1:C:387:PRO:HG3	1.89	0.53
1:C:663:THR:O	1:C:667:ARG:CB	2.51	0.53
1:B:540:LEU:O	1:B:544:THR:HB	2.07	0.53
1:B:684:PRO:HA	1:B:687:PHE:HD2	1.73	0.53
1:D:240:LEU:HD22	1:D:277:ILE:HG12	1.90	0.53
1:D:819:ARG:HA	1:D:822:GLN:HG2	1.91	0.53
1:E:170:GLU:O	1:E:174:GLN:NE2	2.41	0.53
1:F:394:ILE:O	1:F:398:ALA:HB3	2.08	0.53
1:A:783:TYR:HE1	1:A:793:ILE:H	1.55	0.53
1:C:597:PRO:HG3	1:C:694:LEU:HA	1.90	0.53
1:E:350:LEU:HD11	1:E:390:ALA:HB1	1.90	0.53
1:A:183:ARG:NH2	1:A:186:GLU:OE2	2.41	0.53
1:B:366:THR:OG1	1:B:367:ASP:N	2.34	0.53
1:A:368:PRO:O	1:A:372:ALA:HB3	2.09	0.53
1:B:632:ILE:HD11	1:B:662:LEU:HD13	1.90	0.53
1:D:688:ASN:OD1	1:D:750:ARG:NH2	2.39	0.53
1:F:591:LEU:HD13	1:A:827:ASN:HA	1.90	0.53
1:A:628:ALA:HB1	1:A:672:SER:HA	1.91	0.53
1:A:674:ILE:N	1:A:713:VAL:O	2.40	0.53
1:C:738:SER:O	1:C:742:MET:CB	2.56	0.53
1:C:212:LYS:NZ	2:C:901:AGS:S1G	2.82	0.53
1:D:636:GLU:O	1:D:645:ARG:NH2	2.41	0.53
1:F:581:SER:OG	1:F:585:ARG:NH1	2.42	0.53
1:A:738:SER:O	1:A:742:MET:CB	2.56	0.53
1:A:797:ASP:O	1:A:801:LYS:HB2	2.08	0.53
1:D:397:ALA:HA	1:D:539:VAL:HG21	1.91	0.53
1:E:383:ASP:O	1:E:385:GLN:NE2	2.42	0.53
1:B:774:ILE:O	1:B:778:GLN:HB2	2.09	0.53
1:B:819:ARG:HA	1:B:822:GLN:HG2	1.91	0.53
1:C:161:LEU:O	1:C:165:THR:OG1	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ALA:O	1:A:377:SER:CB	2.57	0.52
1:C:774:ILE:O	1:C:778:GLN:HB2	2.09	0.52
1:D:754:ILE:HA	1:D:757:ILE:HG12	1.91	0.52
1:F:783:TYR:O	1:F:787:GLU:HB3	2.09	0.52
1:A:384:ARG:HE	1:A:389:LYS:HB3	1.74	0.52
1:D:318:GLU:O	1:D:322:TYR:CB	2.57	0.52
1:C:199:LYS:NZ	1:D:392:ASP:OD2	2.33	0.52
1:B:676:LEU:HB2	1:B:716:MET:HG2	1.90	0.52
1:E:586:ARG:NH2	1:E:759:GLU:OE2	2.42	0.52
1:F:619:ALA:O	1:F:624:ASP:N	2.43	0.52
1:F:784:LYS:HA	1:F:787:GLU:HG2	1.90	0.52
1:C:327:ALA:HB3	1:D:208:PRO:HD2	1.90	0.52
1:E:631:ARG:HG2	1:E:675:LEU:HD23	1.91	0.52
1:E:738:SER:O	1:E:742:MET:CB	2.55	0.52
1:B:318:GLU:HA	1:B:321:GLN:HB2	1.91	0.52
1:C:652:GLY:H	1:D:654:VAL:HB	1.75	0.52
1:D:240:LEU:HD21	1:D:245:LEU:HD11	1.90	0.52
1:D:575:GLU:O	1:D:579:ALA:HB2	2.09	0.52
1:F:356:ARG:O	1:F:360:HIS:CB	2.57	0.52
1:B:826:GLU:O	1:B:830:ALA:N	2.41	0.52
1:D:377:SER:HB3	1:D:393:LEU:HD12	1.91	0.52
1:D:426:GLN:HA	1:D:429:LEU:HB2	1.90	0.52
1:B:536:ILE:O	1:B:540:LEU:CB	2.58	0.52
1:E:385:GLN:OE1	1:D:331:ARG:NH2	2.43	0.52
1:F:208:PRO:O	1:E:331:ARG:NH2	2.43	0.52
1:C:631:ARG:NH1	1:B:696:ASP:OD2	2.42	0.52
1:F:463:LYS:HD3	1:F:466:LYS:HD3	1.90	0.52
1:B:540:LEU:O	1:B:544:THR:CB	2.57	0.52
1:B:691:LEU:HD21	1:B:750:ARG:HD2	1.92	0.52
1:E:483:LYS:HA	1:E:486:ILE:HG22	1.92	0.52
1:E:724:GLU:OE1	1:E:727:ARG:NH2	2.43	0.52
2:E:901:AGS:O3B	2:E:901:AGS:O2A	2.26	0.52
1:F:619:ALA:HA	1:F:623:PHE:HD2	1.74	0.52
1:E:612:THR:OG1	2:E:902:AGS:O1B	2.28	0.52
1:C:342:SER:OG	1:C:343:VAL:N	2.41	0.51
1:C:583:ALA:HA	1:C:586:ARG:HE	1.74	0.51
1:E:392:ASP:OD2	1:D:199:LYS:NZ	2.42	0.51
1:D:721:GLY:O	1:D:725:THR:HB	2.10	0.51
1:E:745:ILE:HG23	1:E:749:PHE:HB2	1.91	0.51
1:F:347:ILE:HG12	1:F:371:VAL:HA	1.92	0.51
1:F:593:ASP:HB3	1:F:596:ARG:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ARG:HG2	1:A:274:ILE:HG13	1.92	0.51
1:A:380:TYR:HB3	1:A:544:THR:HG21	1.92	0.51
1:E:239:ALA:HA	1:E:276:PHE:HB3	1.93	0.51
1:E:612:THR:N	2:E:902:AGS:O1A	2.39	0.51
1:A:165:THR:OG1	1:A:239:ALA:O	2.21	0.51
1:B:699:LEU:N	1:B:707:VAL:O	2.43	0.51
1:F:251:TYR:CE1	1:A:69:ASN:CA	2.86	0.51
1:A:263:LEU:O	1:A:267:ALA:CB	2.58	0.51
1:B:180:VAL:HB	1:B:183:ARG:HD2	1.91	0.51
1:C:812:TYR:HB3	1:B:755:ASN:HD21	1.75	0.51
1:D:639:GLU:OE1	1:D:645:ARG:NH2	2.43	0.51
1:F:399:SER:OG	1:F:402:ARG:NH2	2.44	0.51
1:F:509:LEU:O	1:F:513:LEU:CB	2.58	0.51
1:A:422:LEU:HD22	1:A:444:LEU:HD11	1.93	0.51
1:D:376:LEU:HB3	1:D:540:LEU:HD22	1.92	0.51
1:E:661:TYR:O	1:E:665:ALA:CB	2.58	0.51
1:A:596:ARG:HH12	1:A:756:ARG:HB3	1.76	0.51
1:B:391:ILE:HG21	2:B:901:AGS:H1'	1.92	0.51
1:C:666:VAL:HG11	1:C:674:ILE:HG12	1.92	0.51
1:D:786:LEU:HA	1:D:791:TYR:HD2	1.76	0.51
1:B:253:GLY:HA2	1:B:256:GLU:HB2	1.93	0.51
1:C:617:ALA:O	1:C:621:PHE:CB	2.51	0.51
1:C:636:GLU:OE1	1:C:645:ARG:NH2	2.43	0.51
1:C:780:LYS:HA	1:C:783:TYR:HD2	1.76	0.51
1:D:771:ILE:HG12	1:D:814:ALA:HB2	1.92	0.51
1:E:256:GLU:O	1:E:260:LYS:HB2	2.11	0.51
1:A:499:SER:O	1:A:503:TYR:HB2	2.11	0.51
1:B:214:ALA:HA	1:B:217:GLU:HG2	1.92	0.51
1:C:318:GLU:O	1:C:322:TYR:CB	2.58	0.51
1:D:605:GLY:HA2	1:D:725:THR:HG21	1.92	0.51
1:A:183:ARG:HD3	1:A:341:PRO:HB3	1.94	0.51
1:A:373:ALA:O	1:A:377:SER:HB3	2.10	0.51
1:C:752:GLU:OE2	2:D:902:AGS:H8	2.11	0.51
1:E:300:LYS:O	1:E:304:ALA:HB2	2.10	0.51
1:A:369:ALA:HB1	1:A:536:ILE:HG13	1.93	0.50
1:B:577:VAL:O	1:B:581:SER:CB	2.59	0.50
1:B:625:SER:OG	1:B:627:GLU:OE1	2.28	0.50
1:B:649:ALA:HB3	1:B:656:TYR:HB2	1.93	0.50
1:B:664:GLU:OE1	1:B:667:ARG:NH2	2.44	0.50
1:C:384:ARG:HB2	1:C:389:LYS:HB3	1.93	0.50
1:E:318:GLU:O	1:E:322:TYR:CB	2.48	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:GLY:O	1:A:272:ASN:ND2	2.44	0.50
1:A:673:VAL:HG22	1:A:713:VAL:HB	1.93	0.50
1:B:177:LEU:HD13	1:B:217:GLU:HB2	1.93	0.50
1:C:451:LYS:O	1:C:455:TYR:CB	2.59	0.50
1:C:738:SER:O	1:C:742:MET:HB2	2.10	0.50
1:D:822:GLN:O	1:D:826:GLU:HB2	2.10	0.50
1:E:256:GLU:O	1:E:260:LYS:CB	2.60	0.50
1:F:831:GLN:O	1:F:835:SER:HB2	2.10	0.50
1:B:196:ARG:HB2	1:B:200:ASN:HA	1.94	0.50
1:C:616:LYS:O	1:C:620:ASN:CB	2.59	0.50
1:D:783:TYR:HA	1:D:786:LEU:HD12	1.94	0.50
1:F:242:MET:HA	1:F:245:LEU:HB2	1.92	0.50
1:A:168:LEU:HA	1:A:171:ARG:HB2	1.94	0.50
1:C:750:ARG:HD2	1:D:607:THR:HG21	1.92	0.50
1:F:472:THR:HA	1:F:475:ILE:HG22	1.94	0.50
1:C:195:GLN:NE2	1:D:400:SER:OG	2.45	0.50
1:E:509:LEU:HA	1:E:512:GLN:HG2	1.94	0.50
1:E:820:ALA:O	1:E:824:GLN:HB2	2.11	0.50
1:B:201:ASN:HB2	1:B:333:PHE:CD1	2.46	0.50
1:F:354:LYS:HA	1:F:357:TYR:HB2	1.92	0.50
1:A:690:LEU:HA	1:A:693:VAL:HG22	1.94	0.50
1:D:283:MET:O	1:D:295:ALA:N	2.45	0.50
1:F:819:ARG:O	1:F:823:GLN:CB	2.60	0.50
1:D:721:GLY:O	1:D:725:THR:CB	2.60	0.50
1:C:747:LYS:O	1:D:723:ARG:NH1	2.44	0.50
1:F:823:GLN:HA	1:F:827:ASN:HD22	1.77	0.50
1:F:586:ARG:HA	1:F:591:LEU:HD12	1.93	0.49
1:B:614:LEU:O	1:B:618:LEU:CB	2.60	0.49
1:B:780:LYS:HA	1:B:783:TYR:HD2	1.76	0.49
1:C:194:LEU:HD22	1:C:309:HIS:HE1	1.76	0.49
1:C:351:ARG:NH2	1:C:367:ASP:OD2	2.41	0.49
1:C:745:ILE:HA	1:C:749:PHE:HD2	1.77	0.49
1:E:668:ARG:HH21	1:D:320:ARG:HH21	1.60	0.49
1:A:584:ILE:HD11	1:A:618:LEU:HD21	1.93	0.49
1:D:679:VAL:HG22	1:D:687:PHE:HE1	1.76	0.49
1:F:822:GLN:HA	1:F:826:GLU:HB2	1.94	0.49
1:C:687:PHE:HD2	1:C:748:ILE:HG12	1.76	0.49
1:E:234:GLY:O	1:E:272:ASN:ND2	2.45	0.49
1:E:368:PRO:HA	1:E:371:VAL:HG12	1.93	0.49
1:C:783:TYR:O	1:C:787:GLU:CB	2.61	0.49
1:F:373:ALA:O	1:F:377:SER:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:409:PRO:HB2	1:F:412:LEU:HD23	1.95	0.49
1:B:341:PRO:HG2	1:B:386:LEU:HB2	1.94	0.49
1:C:600:SER:N	1:C:758:ASP:OD2	2.45	0.49
1:C:631:ARG:HG2	1:C:675:LEU:HD23	1.94	0.49
1:A:565:GLU:HA	1:A:568:HIS:HD1	1.78	0.49
1:C:830:ALA:HA	1:C:833:ILE:HG22	1.95	0.49
1:D:557:GLU:HG3	1:D:561:ARG:HH21	1.78	0.49
1:A:832:GLN:HA	1:A:835:SER:HB3	1.95	0.49
1:B:375:THR:O	1:B:379:ARG:CB	2.60	0.49
1:C:561:ARG:HB2	1:C:564:GLN:HB3	1.95	0.49
1:B:832:GLN:HB3	1:B:838:LEU:HD13	1.94	0.49
1:C:202:PRO:HG2	1:C:311:VAL:HG13	1.95	0.49
1:C:599:GLY:HA3	1:C:713:VAL:HG13	1.95	0.49
1:C:831:GLN:O	1:C:835:SER:CB	2.60	0.49
1:D:165:THR:HG22	1:D:238:LEU:HB3	1.95	0.49
1:D:396:GLU:OE1	1:D:543:TRP:NE1	2.40	0.49
1:D:537:ALA:O	1:D:541:ALA:CB	2.61	0.49
1:A:263:LEU:O	1:A:267:ALA:HB2	2.12	0.49
1:A:620:ASN:HA	1:A:625:SER:H	1.77	0.49
1:B:171:ARG:O	1:B:175:GLY:N	2.46	0.48
1:D:354:LYS:O	1:D:358:GLU:HB2	2.13	0.48
1:D:585:ARG:O	1:D:589:ALA:CB	2.60	0.48
1:E:317:ASP:OD1	1:E:317:ASP:N	2.45	0.48
1:F:252:ARG:HH12	1:A:250:LYS:HD2	1.78	0.48
1:A:774:ILE:HA	1:A:777:ILE:HG12	1.94	0.48
1:D:634:MET:HG3	1:D:679:VAL:HA	1.95	0.48
1:F:235:ARG:HH11	1:F:274:ILE:HD11	1.77	0.48
1:A:405:ILE:HG23	1:A:469:LEU:HD21	1.94	0.48
1:A:661:TYR:O	1:A:665:ALA:CB	2.61	0.48
1:A:738:SER:HB2	1:A:760:VAL:HG11	1.94	0.48
1:D:193:VAL:HG11	1:D:202:PRO:HB3	1.95	0.48
1:F:826:GLU:O	1:F:830:ALA:N	2.43	0.48
1:A:691:LEU:HD21	1:A:750:ARG:HH21	1.78	0.48
1:C:542:ARG:HH12	1:B:189:ARG:HD3	1.78	0.48
1:C:276:PHE:HD1	1:C:311:VAL:HB	1.78	0.48
1:D:780:LYS:HA	1:D:783:TYR:HD2	1.78	0.48
1:F:388:ASP:OD1	1:E:199:LYS:NZ	2.47	0.48
1:C:632:ILE:HD12	1:C:662:LEU:HD12	1.96	0.48
1:C:723:ARG:O	1:C:727:ARG:CB	2.61	0.48
1:E:607:THR:HB	1:E:815:ARG:HD2	1.96	0.48
1:A:769:GLN:O	1:A:773:SER:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:ARG:HD2	1:B:598:ILE:HD13	1.96	0.48
1:C:742:MET:O	1:C:746:LYS:HB2	2.13	0.48
2:D:902:AGS:O1A	2:D:902:AGS:O1B	2.31	0.48
1:C:189:ARG:HG2	1:C:336:VAL:HG13	1.96	0.48
1:C:537:ALA:O	1:C:541:ALA:CB	2.61	0.48
1:B:228:VAL:HG21	1:B:232:LEU:HB2	1.95	0.48
1:C:346:THR:HG21	1:C:386:LEU:HD13	1.96	0.48
1:C:723:ARG:O	1:C:727:ARG:HB2	2.13	0.48
1:D:838:LEU:HG	1:D:857:GLN:HB2	1.95	0.48
1:E:253:GLY:O	1:E:257:GLU:N	2.47	0.48
1:F:620:ASN:HA	1:F:625:SER:H	1.78	0.48
1:F:782:LEU:O	1:F:786:LEU:HB2	2.14	0.48
1:B:634:MET:HG3	1:B:679:VAL:HA	1.95	0.48
1:D:563:GLU:O	1:D:567:HIS:ND1	2.35	0.48
1:D:786:LEU:HB3	1:D:791:TYR:HB2	1.94	0.48
1:E:213:THR:OG1	1:E:278:ASP:OD1	2.32	0.48
1:C:300:LYS:O	1:C:304:ALA:HB2	2.14	0.47
1:C:280:LEU:H	1:C:314:THR:HB	1.79	0.47
1:B:169:THR:HG21	1:B:236:ARG:HB2	1.95	0.47
1:B:280:LEU:HD22	1:B:312:GLY:HA3	1.96	0.47
1:C:585:ARG:O	1:C:589:ALA:CB	2.63	0.47
1:C:678:ALA:HA	1:C:719:ASN:H	1.80	0.47
1:E:509:LEU:O	1:E:513:LEU:CB	2.62	0.47
1:E:647:VAL:HA	1:E:689:ILE:HD13	1.96	0.47
1:E:774:ILE:HA	1:E:777:ILE:HG12	1.96	0.47
1:F:263:LEU:O	1:F:267:ALA:CB	2.62	0.47
1:B:614:LEU:O	1:B:618:LEU:HB3	2.14	0.47
1:C:743:GLU:O	1:C:747:LYS:CB	2.48	0.47
1:D:598:ILE:HB	1:D:713:VAL:HG22	1.95	0.47
1:E:520:GLU:OE1	1:E:529:ASN:ND2	2.45	0.47
1:E:690:LEU:HA	1:E:693:VAL:HG22	1.96	0.47
1:E:850:GLU:O	1:E:852:ARG:N	2.46	0.47
1:F:208:PRO:HG2	1:E:327:ALA:HB2	1.95	0.47
1:F:806:ASN:HB3	1:F:824:GLN:HE22	1.79	0.47
1:F:826:GLU:HA	1:F:829:LEU:HB3	1.95	0.47
1:B:201:ASN:ND2	1:B:310:CYS:SG	2.87	0.47
1:B:368:PRO:HA	1:B:371:VAL:HG12	1.95	0.47
1:C:671:TYR:HA	1:C:712:THR:HB	1.96	0.47
1:F:238:LEU:H	1:F:273:VAL:HG13	1.79	0.47
1:B:198:THR:OG1	1:B:331:ARG:O	2.30	0.47
1:B:815:ARG:HB3	1:A:756:ARG:HH22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:ARG:HG3	1:B:526:LEU:HD12	1.96	0.47
1:A:606:PRO:HD3	1:A:725:THR:HG21	1.97	0.47
1:B:577:VAL:O	1:B:581:SER:HB2	2.15	0.47
1:C:234:GLY:O	1:C:272:ASN:ND2	2.47	0.47
1:D:347:ILE:HG12	1:D:370:ILE:HG22	1.97	0.47
1:D:689:ILE:HG23	1:D:699:LEU:HD13	1.96	0.47
1:E:694:LEU:HD23	1:E:756:ARG:HB2	1.97	0.47
1:F:391:ILE:O	1:F:395:ASP:CB	2.63	0.47
1:F:465:GLU:OE2	1:F:525:ARG:N	2.45	0.47
1:B:302:ALA:O	1:B:308:LEU:N	2.48	0.47
1:C:742:MET:SD	1:D:812:TYR:OH	2.69	0.47
1:E:690:LEU:O	1:E:694:LEU:HB2	2.14	0.47
1:F:644:SER:HA	1:F:647:VAL:HG22	1.96	0.47
1:F:693:VAL:HG22	1:F:709:PHE:HE2	1.80	0.47
1:B:827:ASN:HD22	1:A:586:ARG:HH12	1.63	0.47
1:C:677:ASP:OD1	1:C:717:THR:OG1	2.27	0.47
1:E:600:SER:HB2	1:E:757:ILE:HA	1.97	0.47
1:F:619:ALA:HB1	1:F:628:ALA:HB3	1.96	0.47
1:A:388:ASP:HA	1:A:391:ILE:HD12	1.96	0.47
1:E:689:ILE:HD12	1:E:699:LEU:HD11	1.97	0.47
1:A:573:GLN:HE22	1:A:764:HIS:H	1.62	0.47
1:E:573:GLN:HB3	1:E:576:ALA:HB3	1.97	0.47
1:F:603:PHE:HB2	1:F:717:THR:HG22	1.97	0.47
1:B:698:ARG:HG2	1:B:708:ASP:HA	1.96	0.46
1:E:202:PRO:HG2	1:E:311:VAL:HG13	1.97	0.46
1:A:236:ARG:O	1:A:274:ILE:N	2.48	0.46
1:B:184:ASP:HA	1:B:187:ILE:HG12	1.96	0.46
1:B:831:GLN:O	1:B:835:SER:CB	2.64	0.46
1:C:555:GLU:HG2	1:C:559:LEU:HD23	1.96	0.46
1:E:168:LEU:N	1:E:237:VAL:O	2.40	0.46
1:F:611:LYS:HD2	1:F:717:THR:HG21	1.98	0.46
1:F:633:ASP:HA	1:F:677:ASP:HB2	1.97	0.46
1:B:829:LEU:HD11	1:B:844:ILE:HD13	1.96	0.46
1:E:543:TRP:HE1	1:D:189:ARG:HH12	1.64	0.46
1:E:370:ILE:HG22	1:E:394:ILE:HG13	1.97	0.46
1:F:252:ARG:HE	1:A:23:GLY:C	2.18	0.46
1:A:192:GLN:O	1:A:196:ARG:NH2	2.45	0.46
1:A:300:LYS:O	1:A:304:ALA:CB	2.64	0.46
1:C:613:GLU:HG3	2:C:902:AGS:C4	2.46	0.46
1:D:165:THR:HA	1:D:240:LEU:HA	1.98	0.46
1:E:819:ARG:HH21	1:D:596:ARG:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:605:GLY:H	1:D:721:GLY:HA3	1.80	0.46
1:F:800:LEU:HA	1:F:803:LEU:HD12	1.97	0.46
1:C:368:PRO:HA	1:C:371:VAL:HG12	1.97	0.46
1:C:672:SER:O	1:C:712:THR:OG1	2.33	0.46
1:D:238:LEU:HD13	1:D:273:VAL:HG13	1.97	0.46
1:D:355:GLU:O	1:D:359:LEU:HB2	2.15	0.46
1:F:393:LEU:O	1:F:397:ALA:HB3	2.15	0.46
1:A:274:ILE:HG23	1:A:311:VAL:HG21	1.97	0.46
1:A:201:ASN:O	1:A:334:GLN:N	2.48	0.46
1:E:178:ASP:O	1:E:221:GLN:NE2	2.40	0.46
1:F:585:ARG:O	1:F:589:ALA:CB	2.63	0.46
1:C:533:ASP:O	1:C:537:ALA:HB2	2.15	0.46
1:C:729:SER:HA	1:C:730:ILE:HA	1.63	0.46
1:E:576:ALA:O	1:E:580:VAL:HB	2.15	0.46
1:E:728:LYS:HA	1:E:732:LEU:HB3	1.98	0.46
1:F:499:SER:HB2	1:A:427:GLN:HG3	1.98	0.46
1:B:188:ARG:O	1:B:192:GLN:HB2	2.16	0.46
1:C:211:GLY:O	1:C:215:ILE:N	2.49	0.46
1:D:415:LEU:HD13	1:D:455:TYR:HA	1.97	0.46
1:D:696:ASP:O	1:D:698:ARG:NH1	2.49	0.46
1:D:786:LEU:O	1:D:790:GLY:N	2.45	0.46
1:E:414:ARG:HB3	1:E:418:ARG:HH21	1.81	0.46
1:F:341:PRO:HB2	1:F:345:ASP:HB3	1.98	0.46
1:D:776:GLN:HA	1:D:779:LEU:HD12	1.96	0.46
1:F:280:LEU:HD22	1:F:312:GLY:HA3	1.98	0.46
1:F:767:GLY:O	1:F:771:ILE:N	2.41	0.46
1:A:369:ALA:O	1:A:373:ALA:CB	2.63	0.45
1:A:356:ARG:NH1	1:A:480:GLU:OE2	2.48	0.45
1:B:639:GLU:HG2	1:B:641:HIS:H	1.80	0.45
1:B:819:ARG:NE	1:A:755:ASN:O	2.50	0.45
1:C:573:GLN:HB3	1:C:576:ALA:HB3	1.98	0.45
1:C:575:GLU:O	1:C:579:ALA:HB3	2.15	0.45
1:D:178:ASP:HA	1:D:179:PRO:HD3	1.80	0.45
1:D:661:TYR:O	1:D:665:ALA:CB	2.64	0.45
1:E:585:ARG:O	1:E:589:ALA:CB	2.64	0.45
1:F:221:GLN:HA	1:F:224:ILE:HG22	1.97	0.45
1:B:191:ILE:HA	1:B:194:LEU:HD12	1.99	0.45
1:D:330:GLU:OE2	1:D:331:ARG:NH1	2.48	0.45
1:D:613:GLU:HA	1:D:616:LYS:HE3	1.99	0.45
1:E:451:LYS:O	1:E:455:TYR:HB2	2.16	0.45
1:E:596:ARG:NH2	1:E:758:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ASN:ND2	1:A:310:CYS:O	2.50	0.45
1:A:204:LEU:HB2	1:A:313:ALA:HB1	1.98	0.45
1:A:378:HIS:HB2	1:A:386:LEU:HD21	1.99	0.45
1:A:729:SER:HB2	1:A:765:PRO:HD2	1.99	0.45
1:D:251:TYR:CD1	1:A:74:VAL:C	2.89	0.45
1:D:349:ILE:O	1:D:352:GLY:N	2.49	0.45
1:D:575:GLU:O	1:D:579:ALA:CB	2.64	0.45
1:E:247:ALA:O	1:E:249:ALA:N	2.47	0.45
1:F:357:TYR:HA	1:F:361:HIS:HD2	1.82	0.45
1:F:537:ALA:O	1:F:541:ALA:HB2	2.16	0.45
1:F:616:LYS:O	1:F:620:ASN:HB2	2.16	0.45
1:B:800:LEU:O	1:B:804:SER:CB	2.63	0.45
2:C:902:AGS:O2G	2:C:902:AGS:O1B	2.35	0.45
1:A:444:LEU:O	1:A:448:LEU:CB	2.65	0.45
1:B:303:LEU:HG	1:B:308:LEU:HD23	1.99	0.45
1:C:533:ASP:O	1:C:537:ALA:CB	2.64	0.45
1:E:825:ILE:HG23	1:E:853:ILE:HG21	1.98	0.45
1:A:616:LYS:O	1:A:620:ASN:HB2	2.16	0.45
1:A:820:ALA:O	1:A:824:GLN:HB2	2.16	0.45
1:B:161:LEU:HG	1:B:262:VAL:HA	1.99	0.45
1:B:586:ARG:HA	1:B:591:LEU:HD22	1.98	0.45
1:C:269:GLN:HG3	1:C:273:VAL:HB	1.98	0.45
1:C:299:LEU:O	1:C:303:LEU:N	2.48	0.45
1:C:575:GLU:O	1:C:579:ALA:CB	2.65	0.45
1:C:585:ARG:O	1:C:589:ALA:HB2	2.15	0.45
1:E:606:PRO:HA	1:E:722:VAL:HG13	1.99	0.45
1:F:649:ALA:HB1	1:F:653:TYR:HB2	1.98	0.45
1:F:812:TYR:HB2	1:F:816:PRO:HD3	1.97	0.45
1:C:326:ASP:HB3	1:C:329:LEU:HB2	1.98	0.45
1:A:603:PHE:HB2	1:A:717:THR:HA	1.98	0.45
1:B:166:ILE:HD13	1:A:305:ARG:HH11	1.82	0.45
1:B:240:LEU:HD13	1:B:262:VAL:HG21	1.98	0.45
1:B:599:GLY:HA3	1:B:713:VAL:HA	1.97	0.45
1:F:623:PHE:HB3	1:F:671:TYR:CZ	2.52	0.45
1:F:677:ASP:OD1	1:F:717:THR:OG1	2.34	0.45
1:B:263:LEU:HA	1:B:266:LEU:HD12	1.98	0.45
1:E:687:PHE:HD1	1:E:690:LEU:HD12	1.81	0.45
1:E:687:PHE:O	1:E:750:ARG:NH2	2.50	0.45
1:F:487:GLU:OE2	1:F:490:ARG:NH1	2.49	0.45
1:B:237:VAL:HA	1:B:274:ILE:HB	1.99	0.44
1:B:323:ILE:HA	1:B:323:ILE:HD13	1.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:VAL:HG21	1:B:666:VAL:HG12	1.99	0.44
1:D:376:LEU:O	1:D:380:TYR:HB2	2.17	0.44
1:E:636:GLU:OE1	1:D:700:THR:OG1	2.35	0.44
1:A:193:VAL:HG11	1:A:202:PRO:HB3	1.98	0.44
1:A:195:GLN:HE21	1:A:196:ARG:HH21	1.64	0.44
1:A:320:ARG:NH1	1:A:324:GLU:OE1	2.49	0.44
1:B:796:SER:OG	1:B:797:ASP:N	2.51	0.44
1:E:249:ALA:HB1	1:E:254:GLU:HB3	1.98	0.44
1:F:496:ALA:O	1:F:500:GLU:CB	2.64	0.44
1:C:691:LEU:O	1:C:695:ASP:HB2	2.17	0.44
1:D:567:HIS:CE1	1:D:577:VAL:HG11	2.53	0.44
1:E:213:THR:OG1	2:E:901:AGS:O1B	2.35	0.44
1:A:686:VAL:HA	1:A:689:ILE:HG12	2.00	0.44
1:B:786:LEU:HD22	1:B:793:ILE:HD11	1.98	0.44
1:C:698:ARG:HH11	1:C:710:ARG:HH11	1.66	0.44
1:A:633:ASP:HA	1:A:677:ASP:HB2	2.00	0.44
1:C:668:ARG:HE	1:B:320:ARG:NH1	2.15	0.44
1:B:388:ASP:OD2	1:A:331:ARG:NH2	2.51	0.44
1:E:613:GLU:O	1:E:617:ALA:CB	2.66	0.44
1:A:394:ILE:O	1:A:398:ALA:HB3	2.18	0.44
1:A:509:LEU:O	1:A:513:LEU:CB	2.66	0.44
1:A:821:ILE:HG23	1:A:825:ILE:HD12	2.00	0.44
1:C:260:LYS:HE3	1:D:244:ALA:HA	2.00	0.44
1:C:196:ARG:HG3	1:D:396:GLU:HB2	1.99	0.44
1:A:845:ARG:NH1	1:A:847:GLU:OE2	2.51	0.44
1:B:693:VAL:HG13	1:B:709:PHE:HD2	1.82	0.44
1:C:263:LEU:O	1:C:267:ALA:HB2	2.18	0.44
1:C:555:GLU:HG3	1:C:558:LYS:HE2	2.00	0.44
1:C:650:PRO:HG2	1:D:641:HIS:HB3	1.99	0.44
1:A:241:ASP:O	1:A:245:LEU:N	2.50	0.44
1:A:619:ALA:HB1	1:A:628:ALA:HB3	2.00	0.44
1:C:641:HIS:O	1:C:644:SER:OG	2.30	0.44
1:F:167:ASP:HA	1:F:238:LEU:HA	1.99	0.44
1:A:327:ALA:HA	1:A:330:GLU:HG2	1.98	0.44
1:A:803:LEU:O	1:A:807:GLY:HA3	2.17	0.44
1:C:384:ARG:NH1	1:B:330:GLU:OE2	2.45	0.44
1:F:537:ALA:O	1:F:541:ALA:HB3	2.17	0.44
1:C:377:SER:HB2	1:C:389:LYS:HG3	2.00	0.43
1:C:418:ARG:O	1:C:422:LEU:HB2	2.18	0.43
1:C:439:LYS:HA	1:C:439:LYS:HD3	1.79	0.43
1:F:792:GLU:OE2	1:F:794:HIS:NE2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:O	1:A:200:ASN:ND2	2.45	0.43
1:C:168:LEU:HD22	1:C:217:GLU:HG2	2.00	0.43
1:C:317:ASP:O	1:C:321:GLN:HB2	2.19	0.43
1:D:752:GLU:HA	1:D:755:ASN:HB2	2.00	0.43
1:D:694:LEU:HD13	1:D:756:ARG:HB2	2.00	0.43
1:A:795:ILE:HG12	1:A:846:LEU:HD12	2.00	0.43
1:B:184:ASP:OD1	1:B:222:ARG:NH2	2.37	0.43
1:C:183:ARG:NH2	1:C:341:PRO:HD2	2.33	0.43
1:E:737:ASN:O	1:E:741:ALA:CB	2.63	0.43
1:E:793:ILE:HG12	1:E:844:ILE:HB	1.99	0.43
1:C:183:ARG:HH22	1:C:341:PRO:HD2	1.83	0.43
1:F:791:TYR:HD1	1:F:844:ILE:HD11	1.83	0.43
1:A:195:GLN:HE21	1:A:196:ARG:NH2	2.16	0.43
1:A:631:ARG:HA	1:A:675:LEU:HB3	2.00	0.43
1:A:693:VAL:HG11	1:A:699:LEU:HD12	2.01	0.43
1:B:639:GLU:HG3	1:B:641:HIS:HD2	1.83	0.43
1:C:279:ALA:HB1	1:C:281:HIS:CE1	2.53	0.43
1:C:608:GLY:HA2	1:C:815:ARG:HD2	1.98	0.43
1:D:393:LEU:HD21	1:D:540:LEU:HD13	2.01	0.43
1:A:563:GLU:OE1	1:A:585:ARG:NH2	2.51	0.43
1:B:192:GLN:O	1:B:196:ARG:NE	2.51	0.43
1:D:232:LEU:HA	1:D:235:ARG:HD2	2.01	0.43
1:D:722:VAL:HG13	1:D:723:ARG:HG3	2.01	0.43
1:F:654:VAL:HG22	1:E:652:GLY:HA3	2.01	0.43
1:A:361:HIS:NE2	1:A:395:ASP:OD1	2.43	0.43
1:C:429:LEU:HD23	1:B:351:ARG:HH12	1.83	0.43
1:C:619:ALA:HA	1:C:623:PHE:HD2	1.82	0.43
1:D:208:PRO:O	1:D:385:GLN:NE2	2.47	0.43
1:F:483:LYS:HA	1:F:486:ILE:HG22	2.01	0.43
1:F:627:GLU:HB2	1:F:669:ARG:NH2	2.33	0.43
1:C:619:ALA:O	1:C:624:ASP:N	2.52	0.43
1:D:161:LEU:HD21	1:D:262:VAL:HG13	2.01	0.43
1:D:230:GLU:HA	1:D:233:LYS:HG2	2.00	0.43
1:F:179:PRO:HA	1:F:221:GLN:HE22	1.83	0.43
1:A:161:LEU:HD22	1:A:162:LYS:HZ2	1.84	0.43
1:C:679:VAL:HG21	1:C:690:LEU:HD11	2.01	0.43
1:C:820:ALA:HA	1:C:823:GLN:HG2	2.01	0.43
1:C:751:PRO:HB3	1:D:812:TYR:CD1	2.54	0.42
1:E:167:ASP:HB2	1:E:236:ARG:HH21	1.84	0.42
1:E:803:LEU:HD13	1:E:821:ILE:HG12	2.00	0.42
1:F:742:MET:HA	1:F:745:ILE:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:901:AGS:O1B	2:B:901:AGS:O2G	2.36	0.42
1:C:532:THR:H	1:C:535:GLU:HB2	1.83	0.42
1:C:686:VAL:HA	1:C:689:ILE:HG12	2.01	0.42
1:E:359:LEU:HD23	1:E:480:GLU:HB2	2.01	0.42
1:A:605:GLY:HA3	1:A:606:PRO:HD3	1.84	0.42
1:D:330:GLU:HG3	1:D:331:ARG:HG3	2.00	0.42
1:F:827:ASN:HD21	1:E:586:ARG:HD2	1.83	0.42
1:B:827:ASN:HA	1:B:830:ALA:HB3	2.00	0.42
1:D:573:GLN:HB3	1:D:576:ALA:HB3	2.01	0.42
1:D:728:LYS:HD3	1:D:732:LEU:HD22	2.01	0.42
1:D:803:LEU:HD23	1:D:806:ASN:HD22	1.84	0.42
1:E:207:GLU:HA	1:E:208:PRO:HD3	1.86	0.42
1:E:566:LEU:HD13	1:E:614:LEU:HD11	1.99	0.42
1:F:269:GLN:HG3	1:F:272:ASN:HB3	2.00	0.42
1:F:625:SER:OG	1:F:669:ARG:NH2	2.42	0.42
1:F:560:LEU:HD11	1:A:834:LEU:HB3	2.02	0.42
1:C:299:LEU:HD22	1:C:308:LEU:HD22	2.00	0.42
1:E:661:TYR:O	1:E:665:ALA:HB3	2.20	0.42
1:E:612:THR:OG1	2:E:902:AGS:O3G	2.27	0.42
1:F:585:ARG:O	1:F:589:ALA:HB2	2.19	0.42
1:F:615:CYS:O	1:F:619:ALA:CB	2.68	0.42
1:C:447:GLU:O	1:C:451:LYS:HG2	2.19	0.42
1:D:183:ARG:NH2	1:D:210:VAL:O	2.53	0.42
2:E:902:AGS:O1B	2:E:902:AGS:O2G	2.37	0.42
1:F:238:LEU:HD13	1:F:273:VAL:HG22	2.01	0.42
1:F:408:LYS:HE3	1:F:412:LEU:HB3	2.01	0.42
1:F:619:ALA:HA	1:F:623:PHE:HB2	2.01	0.42
1:F:657:GLU:OE2	1:E:703:GLN:NE2	2.53	0.42
1:A:232:LEU:HD13	1:A:232:LEU:HA	1.94	0.42
1:A:373:ALA:O	1:A:377:SER:OG	2.34	0.42
1:C:222:ARG:HG2	1:C:228:VAL:HB	2.01	0.42
1:C:240:LEU:HD21	1:C:245:LEU:HD11	2.01	0.42
1:F:221:GLN:O	1:F:225:ASN:CB	2.59	0.42
1:A:609:VAL:HG23	1:A:763:PHE:HD2	1.85	0.42
1:A:849:ASN:H	1:A:854:VAL:HG12	1.85	0.42
1:C:629:MET:HG2	1:C:631:ARG:HG3	2.02	0.42
1:C:632:ILE:HD13	1:C:662:LEU:HA	2.02	0.42
1:E:240:LEU:HD22	1:E:275:LEU:HD11	2.01	0.42
1:A:728:LYS:HZ2	1:A:762:VAL:HG11	1.85	0.41
1:A:779:LEU:HD21	1:A:795:ILE:HD12	2.01	0.41
1:B:197:ARG:HG3	1:B:198:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:MET:HA	1:B:745:ILE:HG22	2.01	0.41
1:C:752:GLU:O	1:C:756:ARG:HB2	2.19	0.41
1:E:555:GLU:O	1:E:559:LEU:HB2	2.20	0.41
1:E:729:SER:HA	1:E:730:ILE:HA	1.63	0.41
1:F:395:ASP:OD2	1:E:198:THR:N	2.47	0.41
1:B:212:LYS:HA	1:B:215:ILE:HD12	2.02	0.41
2:B:901:AGS:H5'1	1:A:331:ARG:CZ	2.50	0.41
1:C:203:VAL:N	1:C:334:GLN:O	2.54	0.41
1:C:698:ARG:HD2	1:C:706:THR:HB	2.02	0.41
1:E:388:ASP:HB2	2:E:901:AGS:H8	2.00	0.41
1:F:611:LYS:HB3	1:F:675:LEU:HD11	2.00	0.41
1:A:415:LEU:HD13	1:A:418:ARG:HD2	2.02	0.41
1:B:599:GLY:HA3	1:B:714:VAL:H	1.85	0.41
1:F:804:SER:O	1:F:808:TYR:N	2.51	0.41
1:A:733:ILE:HG22	1:A:735:GLN:H	1.86	0.41
1:A:828:PRO:HA	1:A:831:GLN:HB3	2.02	0.41
1:B:533:ASP:OD1	1:B:533:ASP:N	2.53	0.41
1:D:537:ALA:O	1:D:541:ALA:HB3	2.21	0.41
1:F:422:LEU:HD22	1:F:448:LEU:HD23	2.03	0.41
1:F:628:ALA:HB2	1:F:669:ARG:HE	1.86	0.41
1:D:171:ARG:HA	1:D:176:LYS:HE3	2.02	0.41
1:F:538:GLU:HB3	1:F:542:ARG:HH21	1.85	0.41
1:A:224:ILE:O	1:A:233:LYS:NZ	2.53	0.41
1:B:178:ASP:HA	1:B:179:PRO:HD3	1.90	0.41
1:C:356:ARG:O	1:C:360:HIS:HB2	2.20	0.41
1:C:524:MET:HB2	1:C:527:LEU:HG	2.03	0.41
1:D:577:VAL:O	1:D:581:SER:CB	2.69	0.41
1:D:212:LYS:NZ	2:D:901:AGS:O1B	2.50	0.41
1:E:251:TYR:CE1	1:A:72:PRO:C	2.87	0.41
1:E:327:ALA:HA	1:E:330:GLU:HG2	2.02	0.41
1:F:164:TYR:CZ	1:F:258:ARG:HD3	2.55	0.41
1:F:204:LEU:H	1:F:313:ALA:HA	1.85	0.41
1:F:166:ILE:O	1:F:239:ALA:N	2.39	0.41
1:A:226:GLY:HA2	1:A:233:LYS:HD2	2.03	0.41
1:B:314:THR:HG23	1:B:319:TYR:HB2	2.03	0.41
1:C:702:GLY:HA2	1:D:645:ARG:HH11	1.85	0.41
1:F:405:ILE:HD11	1:F:529:ASN:HA	2.03	0.41
1:F:794:HIS:N	1:F:844:ILE:O	2.38	0.41
1:A:381:ILE:HG22	1:A:384:ARG:H	1.86	0.41
1:A:566:LEU:HD13	1:A:614:LEU:HD11	2.03	0.41
1:C:194:LEU:HD11	1:C:219:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:607:THR:HG22	1:D:815:ARG:HH22	1.86	0.41
1:F:610:GLY:O	1:F:614:LEU:N	2.52	0.41
1:F:676:LEU:HB2	1:F:716:MET:HA	2.02	0.41
1:F:793:ILE:HA	1:F:844:ILE:HB	2.02	0.41
1:A:174:GLN:HB3	1:A:176:LYS:HG3	2.02	0.41
1:A:297:ASN:HA	1:A:300:LYS:HE3	2.03	0.41
1:B:357:TYR:OH	2:B:901:AGS:O2'	2.39	0.41
1:C:280:LEU:HD13	1:C:312:GLY:HA2	2.03	0.41
1:D:546:ILE:HG21	1:D:588:ARG:HH12	1.86	0.41
1:E:800:LEU:HA	1:E:803:LEU:HD12	2.03	0.41
1:F:305:ARG:HH21	1:A:244:ALA:HB2	1.86	0.41
1:F:350:LEU:HB2	1:F:370:ILE:HG23	2.03	0.41
1:F:355:GLU:O	1:F:359:LEU:HB2	2.20	0.41
1:F:604:LEU:HD23	1:F:718:SER:HB3	2.03	0.41
1:A:533:ASP:N	1:A:533:ASP:OD1	2.53	0.41
1:B:397:ALA:O	1:B:401:ILE:HG12	2.21	0.41
1:C:399:SER:HA	1:C:402:ARG:HH21	1.86	0.41
1:F:835:SER:HA	1:E:556:ARG:HG3	2.03	0.41
1:F:319:TYR:CE2	1:F:335:LYS:HG2	2.56	0.41
1:F:834:LEU:HB3	1:E:556:ARG:NH1	2.36	0.41
1:B:548:VAL:HG11	1:B:551:MET:HG2	2.03	0.40
1:C:183:ARG:NH2	1:C:339:ALA:O	2.53	0.40
1:C:388:ASP:HA	1:C:391:ILE:HD12	2.02	0.40
1:C:655:GLY:O	1:C:659:GLY:N	2.55	0.40
1:D:663:THR:O	1:D:667:ARG:CB	2.66	0.40
1:C:530:LYS:HB3	1:C:532:THR:HG23	2.03	0.40
1:C:758:ASP:HA	1:D:819:ARG:NH2	2.36	0.40
1:C:839:VAL:HB	1:C:842:LYS:HD3	2.03	0.40
1:C:695:ASP:OD2	2:D:902:AGS:O3G	2.38	0.40
1:E:314:THR:OG1	1:E:315:THR:N	2.50	0.40
1:E:815:ARG:HH22	2:E:902:AGS:H5'1	1.86	0.40
1:D:229:PRO:O	1:D:233:LYS:N	2.50	0.40
1:F:642:SER:HA	1:F:645:ARG:HE	1.87	0.40
1:A:486:ILE:HD12	1:A:486:ILE:HA	1.98	0.40
1:B:606:PRO:HA	1:B:722:VAL:HG13	2.03	0.40
1:C:411:GLU:HA	1:C:414:ARG:HD3	2.04	0.40
1:C:607:THR:OG1	1:C:726:GLU:OE2	2.29	0.40
1:E:639:GLU:HG3	1:E:641:HIS:HB2	2.04	0.40
1:F:192:GLN:HG3	1:A:400:SER:HB2	2.03	0.40
1:F:202:PRO:HD2	1:F:311:VAL:HA	2.02	0.40
1:B:698:ARG:HB3	1:B:699:LEU:H	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:821:ILE:HG23	1:C:825:ILE:HD12	2.02	0.40
1:D:300:LYS:O	1:D:304:ALA:CB	2.70	0.40
1:E:332:ARG:HD3	1:E:332:ARG:HA	1.95	0.40
1:F:230:GLU:HG3	1:A:407:SER:HA	2.03	0.40
1:F:483:LYS:HA	1:F:483:LYS:HD3	1.98	0.40
1:F:773:SER:HA	1:F:776:GLN:HG2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	811/871 (93%)	764 (94%)	47 (6%)	0	100	100
1	B	566/871 (65%)	520 (92%)	45 (8%)	1 (0%)	51	85
1	C	618/871 (71%)	560 (91%)	58 (9%)	0	100	100
1	D	618/871 (71%)	572 (93%)	46 (7%)	0	100	100
1	E	682/871 (78%)	637 (93%)	45 (7%)	0	100	100
1	F	682/871 (78%)	630 (92%)	52 (8%)	0	100	100
All	All	3977/5226 (76%)	3683 (93%)	293 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	323	ILE

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

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	582/726 (80%)	574 (99%)	8 (1%)	71	86
1	B	483/726 (66%)	474 (98%)	9 (2%)	62	82
1	C	533/726 (73%)	527 (99%)	6 (1%)	78	89
1	D	533/726 (73%)	522 (98%)	11 (2%)	59	80
1	E	582/726 (80%)	576 (99%)	6 (1%)	80	90
1	F	582/726 (80%)	572 (98%)	10 (2%)	66	84
All	All	3295/4356 (76%)	3245 (98%)	50 (2%)	72	86

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	268	LYS
1	C	272	ASN
1	C	297	ASN
1	C	441	LEU
1	C	620	ASN
1	C	643	VAL
1	F	268	LYS
1	F	401	ILE
1	F	440	ARG
1	F	443	MET
1	F	620	ASN
1	F	638	MET
1	F	646	LEU
1	F	705	ARG
1	F	737	ASN
1	F	845	ARG
1	E	268	LYS
1	E	272	ASN
1	E	297	ASN
1	E	530	LYS
1	E	586	ARG
1	E	620	ASN
1	D	197	ARG
1	D	268	LYS
1	D	401	ILE
1	D	432	GLU

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Mol	Chain	Res	Type
1	D	440	ARG
1	D	443	MET
1	D	620	ASN
1	D	681	LYS
1	D	705	ARG
1	D	737	ASN
1	D	845	ARG
1	B	212	LYS
1	B	252	ARG
1	B	335	LYS
1	B	528	ARG
1	B	530	LYS
1	B	646	LEU
1	B	668	ARG
1	B	737	ASN
1	B	845	ARG
1	A	162	LYS
1	A	272	ASN
1	A	297	ASN
1	A	479	LEU
1	A	530	LYS
1	A	586	ARG
1	A	620	ASN
1	A	646	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	174	GLN
1	C	195	GLN
1	C	269	GLN
1	C	272	ASN
1	C	421	GLN
1	C	688	ASN
1	C	755	ASN
1	C	778	GLN
1	F	361	HIS
1	F	385	GLN
1	F	512	GLN
1	F	529	ASN
1	F	703	GLN
1	F	778	GLN

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Mol	Chain	Res	Type
1	E	174	GLN
1	E	195	GLN
1	E	272	ASN
1	E	620	ASN
1	E	703	GLN
1	E	711	ASN
1	E	770	HIS
1	D	703	GLN
1	D	719	ASN
1	D	737	ASN
1	D	778	GLN
1	D	806	ASN
1	D	822	GLN
1	B	192	GLN
1	B	201	ASN
1	B	641	HIS
1	B	683	HIS
1	B	711	ASN
1	B	737	ASN
1	B	755	ASN
1	B	778	GLN
1	B	849	ASN
1	A	195	GLN
1	A	272	ASN
1	A	620	ASN
1	A	703	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 carbohydrates in this entry.



## 5.6 Ligand geometry

7 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	AGS	B	901	-	26,33,33	0.81	1 (3%)	22,52,52	0.89	1 (4%)
2	AGS	C	901	-	26,33,33	0.74	1 (3%)	22,52,52	1.35	3 (13%)
2	AGS	C	902	-	26,33,33	0.82	1 (3%)	22,52,52	1.14	1 (4%)
2	AGS	D	901	-	26,33,33	0.80	1 (3%)	22,52,52	1.06	1 (4%)
2	AGS	D	902	-	26,33,33	0.80	1 (3%)	22,52,52	1.13	1 (4%)
2	AGS	E	901	-	26,33,33	0.76	1 (3%)	22,52,52	1.38	2 (9%)
2	AGS	E	902	-	26,33,33	0.75	1 (3%)	22,52,52	1.54	2 (9%)

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	AGS	B	901	-	-	0/17/38/38	0/3/3/3
2	AGS	C	901	-	-	0/17/38/38	0/3/3/3
2	AGS	C	902	-	-	0/17/38/38	0/3/3/3
2	AGS	D	901	-	-	0/17/38/38	0/3/3/3
2	AGS	D	902	-	-	0/17/38/38	0/3/3/3
2	AGS	E	901	-	-	0/17/38/38	0/3/3/3
2	AGS	E	902	-	-	0/17/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	AGS	PG-S1G	2.29	1.95	1.90
2	E	902	AGS	PG-S1G	2.30	1.95	1.90
2	C	902	AGS	PG-S1G	2.43	1.95	1.90
2	D	901	AGS	PG-S1G	2.43	1.95	1.90
2	E	901	AGS	PG-S1G	2.48	1.95	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	902	AGS	PG-S1G	2.49	1.95	1.90
2	B	901	AGS	PG-S1G	2.71	1.95	1.90

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	902	AGS	PB-O3B-PG	-6.01	112.94	132.35
2	C	902	AGS	PB-O3B-PG	-4.67	117.24	132.35
2	E	901	AGS	PB-O3B-PG	-4.44	117.98	132.35
2	D	902	AGS	PB-O3B-PG	-4.32	118.39	132.35
2	D	901	AGS	PB-O3B-PG	-4.15	118.93	132.35
2	C	901	AGS	PB-O3B-PG	-4.02	119.35	132.35
2	E	902	AGS	C4'-O4'-C1'	-2.68	106.92	109.77
2	B	901	AGS	PB-O3B-PG	-2.36	124.72	132.35
2	C	901	AGS	C4'-O4'-C1'	-2.06	107.58	109.77
2	C	901	AGS	C1'-N9-C4	3.42	132.54	126.64
2	E	901	AGS	C1'-N9-C4	3.80	133.20	126.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	AGS	4	0
2	C	901	AGS	2	0
2	C	902	AGS	2	0
2	D	901	AGS	1	0
2	D	902	AGS	4	0
2	E	901	AGS	4	0
2	E	902	AGS	6	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.