



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:51 PM BST

PDB ID : 3J9P
EMDB ID: : EMD-6267
Title : Structure of the TRPA1 ion channel determined by electron cryo-microscopy
Authors : Paulsen, C.E.; Armache, J.-P.; Gao, Y.; Cheng, Y.; Julius, D.
Deposited on : 2015-02-14
Resolution : 4.24 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

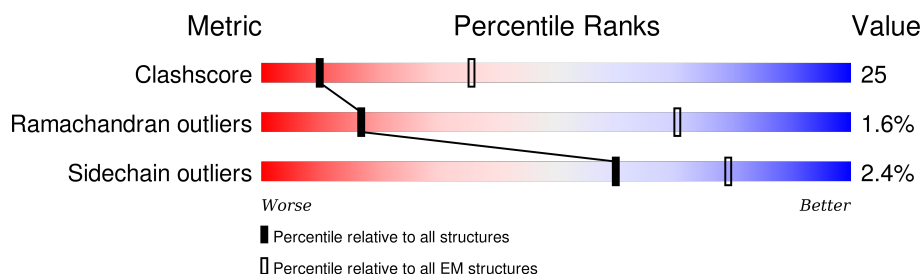
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.24 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 ≥ 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	1528	20% 15% • 63%
1	B	1528	20% 15% • 63%
1	C	1528	20% 15% • 63%
1	D	1528	19% 16% • 63%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16952 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 Maltose-binding periplasmic protein, Transient receptor potential cation channel subfamily A member 1 chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	560	Total	C	N	O	S	0	0
			4238	2775	711	722	30		
1	A	560	Total	C	N	O	S	0	0
			4238	2775	711	722	30		
1	B	560	Total	C	N	O	S	0	0
			4238	2775	711	722	30		
1	C	560	Total	C	N	O	S	0	0
			4238	2775	711	722	30		

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-408	MET	-	EXPRESSION TAG	UNP P0AEX9
D	-407	GLY	-	EXPRESSION TAG	UNP P0AEX9
D	-406	SER	-	EXPRESSION TAG	UNP P0AEX9
D	-405	SER	-	EXPRESSION TAG	UNP P0AEX9
D	-404	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-403	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-402	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-401	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-400	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-399	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-398	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-397	HIS	-	EXPRESSION TAG	UNP P0AEX9
D	-396	GLY	-	EXPRESSION TAG	UNP P0AEX9
D	-395	SER	-	EXPRESSION TAG	UNP P0AEX9
D	-394	SER	-	EXPRESSION TAG	UNP P0AEX9
D	-393	MET	-	EXPRESSION TAG	UNP P0AEX9
D	-26	ASN	-	LINKER	UNP O75762
D	-25	SER	-	LINKER	UNP O75762
D	-24	SER	-	LINKER	UNP O75762
D	-23	SER	-	LINKER	UNP O75762
D	-22	ASN	-	LINKER	UNP O75762

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-21	ASN	-	LINKER	UNP O75762
D	-20	ASN	-	LINKER	UNP O75762
D	-19	ASN	-	LINKER	UNP O75762
D	-18	ASN	-	LINKER	UNP O75762
D	-17	ASN	-	LINKER	UNP O75762
D	-16	ASN	-	LINKER	UNP O75762
D	-15	ASN	-	LINKER	UNP O75762
D	-14	ASN	-	LINKER	UNP O75762
D	-13	ASN	-	LINKER	UNP O75762
D	-12	LEU	-	LINKER	UNP O75762
D	-11	GLY	-	LINKER	UNP O75762
D	-10	ILE	-	LINKER	UNP O75762
D	-9	GLU	-	LINKER	UNP O75762
D	-8	GLU	-	LINKER	UNP O75762
D	-7	ASN	-	LINKER	UNP O75762
D	-6	LEU	-	LINKER	UNP O75762
D	-5	TYR	-	LINKER	UNP O75762
D	-4	PHE	-	LINKER	UNP O75762
D	-3	GLN	-	LINKER	UNP O75762
D	-2	GLY	-	LINKER	UNP O75762
D	-1	ALA	-	LINKER	UNP O75762
D	0	GLY	-	LINKER	UNP O75762
D	1	SER	-	LINKER	UNP O75762
D	966	ASP	GLU	CONFLICT	UNP O75762
A	-408	MET	-	EXPRESSION TAG	UNP P0AEX9
A	-407	GLY	-	EXPRESSION TAG	UNP P0AEX9
A	-406	SER	-	EXPRESSION TAG	UNP P0AEX9
A	-405	SER	-	EXPRESSION TAG	UNP P0AEX9
A	-404	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-403	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-402	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-401	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-400	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-399	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-398	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-397	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-396	GLY	-	EXPRESSION TAG	UNP P0AEX9
A	-395	SER	-	EXPRESSION TAG	UNP P0AEX9
A	-394	SER	-	EXPRESSION TAG	UNP P0AEX9
A	-393	MET	-	EXPRESSION TAG	UNP P0AEX9
A	-26	ASN	-	LINKER	UNP O75762
A	-25	SER	-	LINKER	UNP O75762

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	SER	-	LINKER	UNP O75762
A	-23	SER	-	LINKER	UNP O75762
A	-22	ASN	-	LINKER	UNP O75762
A	-21	ASN	-	LINKER	UNP O75762
A	-20	ASN	-	LINKER	UNP O75762
A	-19	ASN	-	LINKER	UNP O75762
A	-18	ASN	-	LINKER	UNP O75762
A	-17	ASN	-	LINKER	UNP O75762
A	-16	ASN	-	LINKER	UNP O75762
A	-15	ASN	-	LINKER	UNP O75762
A	-14	ASN	-	LINKER	UNP O75762
A	-13	ASN	-	LINKER	UNP O75762
A	-12	LEU	-	LINKER	UNP O75762
A	-11	GLY	-	LINKER	UNP O75762
A	-10	ILE	-	LINKER	UNP O75762
A	-9	GLU	-	LINKER	UNP O75762
A	-8	GLU	-	LINKER	UNP O75762
A	-7	ASN	-	LINKER	UNP O75762
A	-6	LEU	-	LINKER	UNP O75762
A	-5	TYR	-	LINKER	UNP O75762
A	-4	PHE	-	LINKER	UNP O75762
A	-3	GLN	-	LINKER	UNP O75762
A	-2	GLY	-	LINKER	UNP O75762
A	-1	ALA	-	LINKER	UNP O75762
A	0	GLY	-	LINKER	UNP O75762
A	1	SER	-	LINKER	UNP O75762
A	966	ASP	GLU	CONFLICT	UNP O75762
B	-408	MET	-	EXPRESSION TAG	UNP P0AEX9
B	-407	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	-406	SER	-	EXPRESSION TAG	UNP P0AEX9
B	-405	SER	-	EXPRESSION TAG	UNP P0AEX9
B	-404	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-403	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-402	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-401	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-400	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-399	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-398	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-397	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-396	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	-395	SER	-	EXPRESSION TAG	UNP P0AEX9
B	-394	SER	-	EXPRESSION TAG	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-393	MET	-	EXPRESSION TAG	UNP P0AEX9
B	-26	ASN	-	LINKER	UNP O75762
B	-25	SER	-	LINKER	UNP O75762
B	-24	SER	-	LINKER	UNP O75762
B	-23	SER	-	LINKER	UNP O75762
B	-22	ASN	-	LINKER	UNP O75762
B	-21	ASN	-	LINKER	UNP O75762
B	-20	ASN	-	LINKER	UNP O75762
B	-19	ASN	-	LINKER	UNP O75762
B	-18	ASN	-	LINKER	UNP O75762
B	-17	ASN	-	LINKER	UNP O75762
B	-16	ASN	-	LINKER	UNP O75762
B	-15	ASN	-	LINKER	UNP O75762
B	-14	ASN	-	LINKER	UNP O75762
B	-13	ASN	-	LINKER	UNP O75762
B	-12	LEU	-	LINKER	UNP O75762
B	-11	GLY	-	LINKER	UNP O75762
B	-10	ILE	-	LINKER	UNP O75762
B	-9	GLU	-	LINKER	UNP O75762
B	-8	GLU	-	LINKER	UNP O75762
B	-7	ASN	-	LINKER	UNP O75762
B	-6	LEU	-	LINKER	UNP O75762
B	-5	TYR	-	LINKER	UNP O75762
B	-4	PHE	-	LINKER	UNP O75762
B	-3	GLN	-	LINKER	UNP O75762
B	-2	GLY	-	LINKER	UNP O75762
B	-1	ALA	-	LINKER	UNP O75762
B	0	GLY	-	LINKER	UNP O75762
B	1	SER	-	LINKER	UNP O75762
B	966	ASP	GLU	CONFLICT	UNP O75762
C	-408	MET	-	EXPRESSION TAG	UNP P0AEX9
C	-407	GLY	-	EXPRESSION TAG	UNP P0AEX9
C	-406	SER	-	EXPRESSION TAG	UNP P0AEX9
C	-405	SER	-	EXPRESSION TAG	UNP P0AEX9
C	-404	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-403	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-402	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-401	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-400	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-399	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-398	HIS	-	EXPRESSION TAG	UNP P0AEX9
C	-397	HIS	-	EXPRESSION TAG	UNP P0AEX9

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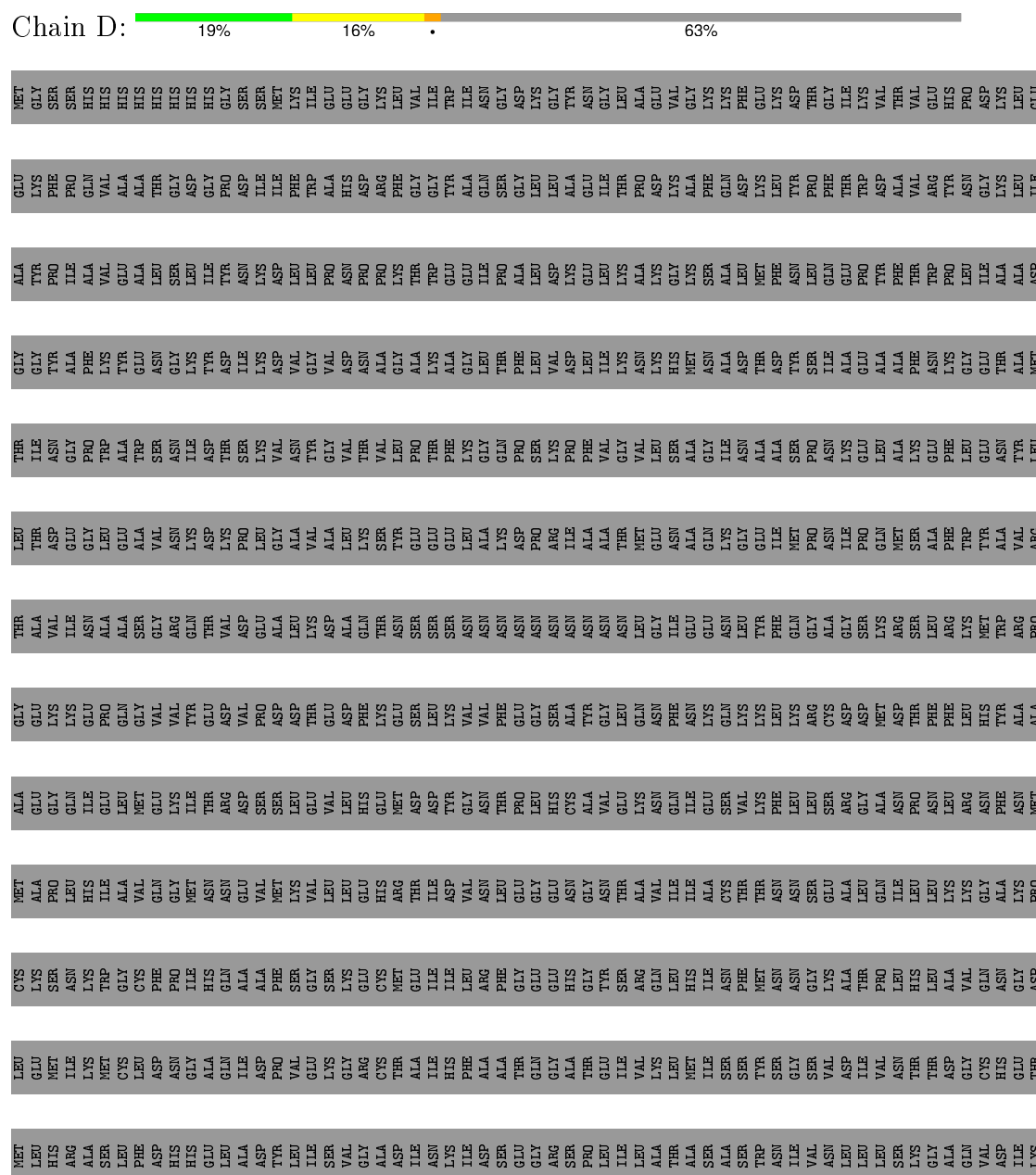
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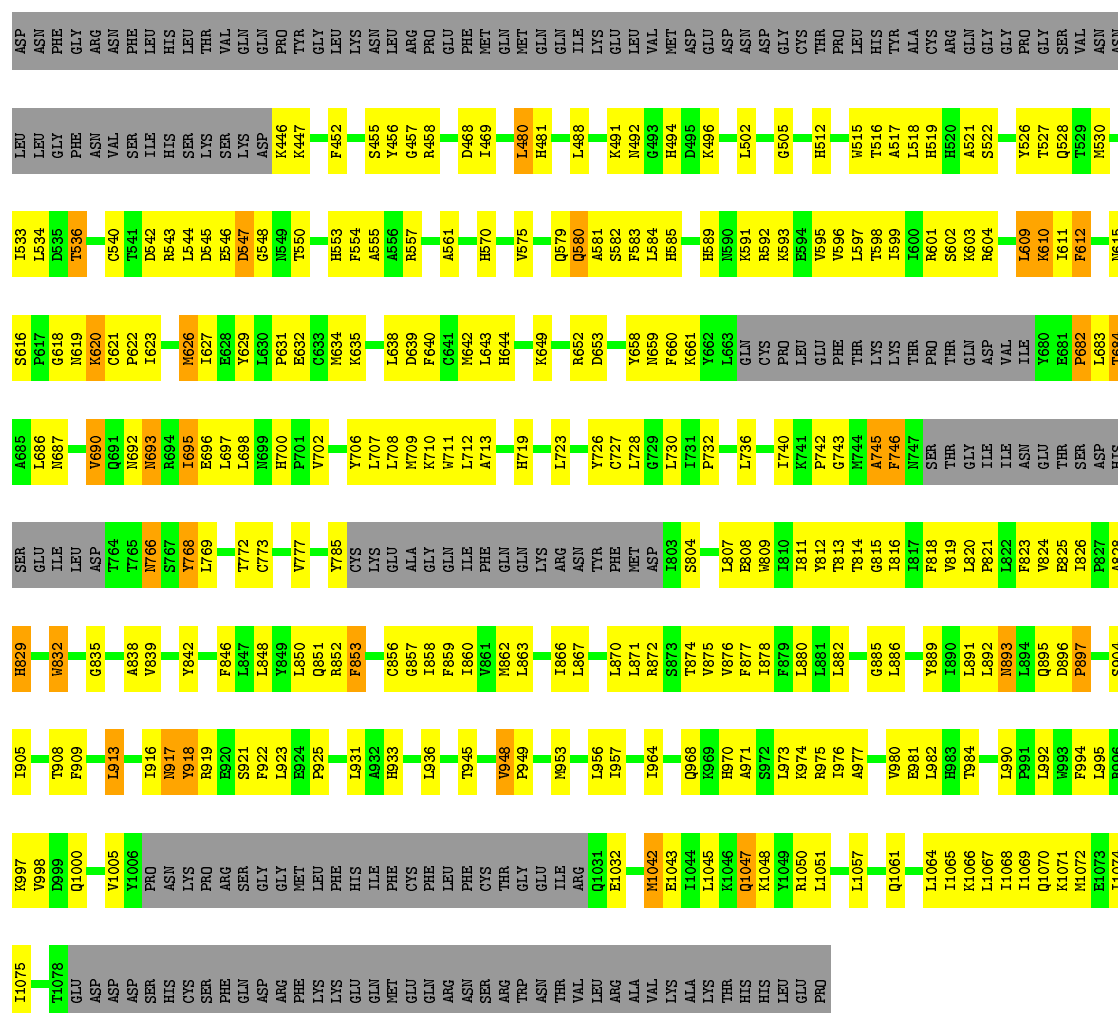
Chain	Residue	Modelled	Actual	Comment	Reference
C	-396	GLY	-	EXPRESSION TAG	UNP P0AEX9
C	-395	SER	-	EXPRESSION TAG	UNP P0AEX9
C	-394	SER	-	EXPRESSION TAG	UNP P0AEX9
C	-393	MET	-	EXPRESSION TAG	UNP P0AEX9
C	-26	ASN	-	LINKER	UNP O75762
C	-25	SER	-	LINKER	UNP O75762
C	-24	SER	-	LINKER	UNP O75762
C	-23	SER	-	LINKER	UNP O75762
C	-22	ASN	-	LINKER	UNP O75762
C	-21	ASN	-	LINKER	UNP O75762
C	-20	ASN	-	LINKER	UNP O75762
C	-19	ASN	-	LINKER	UNP O75762
C	-18	ASN	-	LINKER	UNP O75762
C	-17	ASN	-	LINKER	UNP O75762
C	-16	ASN	-	LINKER	UNP O75762
C	-15	ASN	-	LINKER	UNP O75762
C	-14	ASN	-	LINKER	UNP O75762
C	-13	ASN	-	LINKER	UNP O75762
C	-12	LEU	-	LINKER	UNP O75762
C	-11	GLY	-	LINKER	UNP O75762
C	-10	ILE	-	LINKER	UNP O75762
C	-9	GLU	-	LINKER	UNP O75762
C	-8	GLU	-	LINKER	UNP O75762
C	-7	ASN	-	LINKER	UNP O75762
C	-6	LEU	-	LINKER	UNP O75762
C	-5	TYR	-	LINKER	UNP O75762
C	-4	PHE	-	LINKER	UNP O75762
C	-3	GLN	-	LINKER	UNP O75762
C	-2	GLY	-	LINKER	UNP O75762
C	-1	ALA	-	LINKER	UNP O75762
C	0	GLY	-	LINKER	UNP O75762
C	1	SER	-	LINKER	UNP O75762
C	966	ASP	GLU	CONFLICT	UNP O75762

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

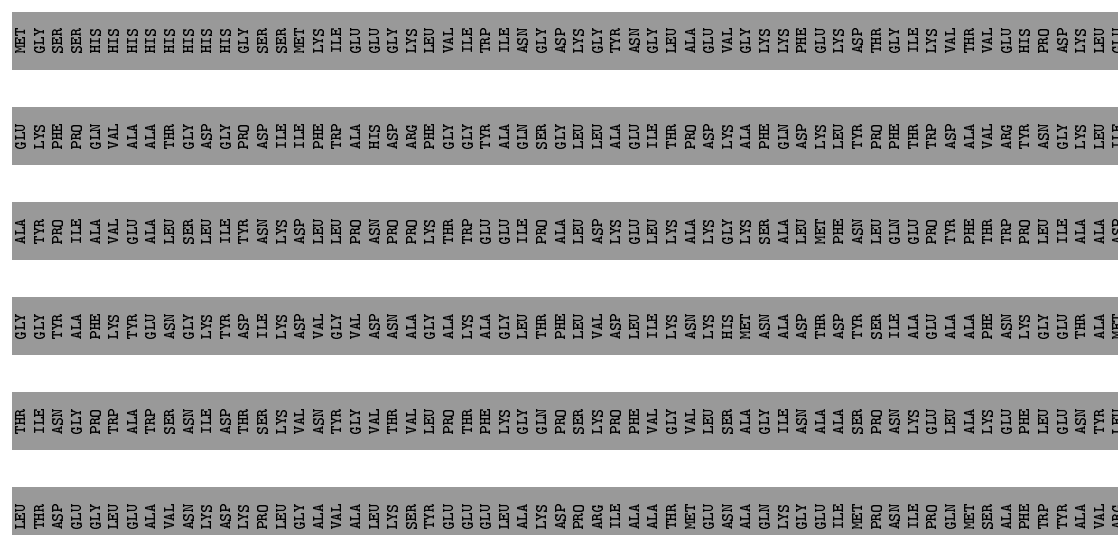
- Molecule 1: Maltose-binding periplasmic protein, Transient receptor potential cation channel subfamily A member 1 chimera





- Molecule 1: Maltose-binding periplasmic protein, Transient receptor potential cation channel subfamily A member 1 chimera

Chain A: 20% 15% 63%



- Molecule 1: Maltose-binding periplasmic protein, Transient receptor potential cation channel subfamily A member 1 chimera

Chain B:		<div><div></div><div></div><div></div></div>		20%	15%	•	63%																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
6618	6619	6620	6621	6622	6623	6624	6625	6626	6627	6628	6629	6630	6631	6632	6633	6634	6635	6636	6637	6638	6639	6640	6641	6642	6643	6644	6645	6646	6647	6648	6649	6650	6651	6652	6653	6654	6655	6656	6657	6658	6659	6660	6661	6662	6663	6664	6665	6666	6667	6668	6669	6670	6671	6672	6673	6674	6675	6676	6677	6678	6679	6680	6681	6682	6683	6684	6685	6686	6687	6688	6689	6690	6691	6692	6693	6694	6695	6696	6697	6698	6699	6700	6701	6702	6703	6704	6705	6706	6707	6708	6709	6710	6711	6712	6713	6714	6715	6716	6717	6718	6719	6720	6721	6722	6723	6724	6725	6726	6727	6728	6729	6730	6731	6732	6733	6734	6735	6736	6737	6738	6739	6740	6741	6742	6743	6744	6745	6746	6747	6748	6749	6750	6751	6752	6753	6754	6755	6756	6757	6758	6759	6760	6761	6762	6763	6764	6765	6766	6767	6768	6769	6770	6771	6772	6773	6774	6775	6776	6777	6778	6779	6780	6781	6782	6783	6784	6785	6786	6787	6788	6789	6790	6791	6792	6793	6794	6795	6796	6797	6798	6799	6800	6801	6802	6803	6804	6805	6806	6807	6808	6809	6810	6811	6812	6813	6814	6815	6816	6817	6818	6819	6820	6821	6822	6823	6824	6825	6826	6827	6828	6829	6830	6831	6832	6833	6834	6835	6836	6837	6838	6839	6840	6841	6842	6843	6844	6845	6846	6847	6848	6849	6850	6851	6852	6853	6854	6855	6856	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	7767	7768	7769	7770	7771	7772	7773	7774	7775	7776	7777	7778	7779	7780	7781	7782	7783	7784	7785	7786	7787	7788	7789	7790	7791	7792	7793	7794	7795	7796	7797	7798	7799	7800	7801	7802	7803	7804	7805	7806	7807	7808	7809	7810	7811	7812	7813	7814	7815	7816	7817	7818	7819	7820	7821	7822	7823	7824	7825	7826	7827	7828	7829	7830	7831	7832	7833	7834	7835	7836	7837	7838	7839	7840	7841	7842	7843	7844	7845	7846	7847	7848	7849	7850	7851	7852	7853	7854	7855	7856	7857	7858	7859	7860	7861	7862	7863	7864	7865	7866	7867	7868	7869	7870	7871	7872	7873	7874	7875	7876	7877	7878	7879	7880	7881	7882	7883	7884	7885	7886	7887	7888	7889	7890	7891	7892	7893	7894	7895	7896	7897	7898	7899	7900	7901	7902	7903	7904	7905	7906	7907	7908	7909	7910	7911	7912	7913	7914	7915	7916	7917	7918	7919	7920	7921	7922	7923	7924	7925	7926	7927	7928	7929	7930	7931	7932	7933	7934	7935	7936	7937	7938	7939	7940	7941	7942	7943	7944	7945	7946	7947	7948	7949	7950	7951	7952	7953	7954	7955	7956	7957	7958	7959	7960	7961	7962	7963	7964	7965	7966	7967	7968	7969	7970	7971	7972	7973

T1078	V998	H929	SER	A695	C618	I533	LEU	ASP	MET	LEU	CYS
GLU	D999	W832	GLU	L666	M619	L534	LEU	ASN	LEU	GLU	LYS
ASP	Q1000	W832	ILE	M637	K620	D535	GLY	PHE	HIS	MET	SER
ASP	V1005	G835	ASP	V690	C621	T536	ASN	ARG	ALA	LYS	TRP
ASP	V1006	G835	ASP	G691	I623	C540	VAL	ASN	SER	MET	GLY
PRO	PRO	W839	T764	M692	I623	T541	SER	PHE	LEU	CYS	CYS
ASN	ASN	Y817	T765	M693	W626	D542	ILE	LEU	ASP	LEU	PHE
LYS	LYS	Y842	N766	M694	I627	D543	HIS	HIS	ASP	ASP	PRO
PRO	PRO	Y842	S767	M694	E628	L544	SER	LEU	HIS	ASN	ILE
ARG	ARG	F846	Y769	E696	Y629	D545	THR	THR	HIS	GLY	ALA
SER	SER	F846	L769	L697	L630	E546	SER	VAL	GLU	ALA	HIS
GLY	GLY	L848	T772	L698	L631	D547	LYS	GLN	LEU	GLN	ALA
ASP	ASP	W649	C773	M699	E632	G548	ASP	GLN	ALA	ILE	ALA
GLY	GLY	L823	C773	E632	E633	G549	ASP	PRO	ASP	ASP	ALA
ARG	ARG	L823	C773	E632	C634	T550	ASP	TYR	TYR	PRO	PHE
PHE	PHE	L850	V777	H700	M634	T550	VAL	LEU	VAL	VAL	SER
LEU	LEU	Q851	V777	F701	M634	T550	GLY	GLY	LEU	GLY	GLY
LYS	LYS	R852	V702	V702	K635	F452	ILE	ILE	ILE	LYS	SER
PHE	PHE	F853	Y785	Y706	K635	F452	LYS	LYS	SER	LYS	SER
HIS	HIS	F853	CYS	L638	L638	F554	ASN	ASN	VAL	GLY	LYS
GLU	GLU	F853	LYS	D639	D639	F554	LEU	LEU	VAL	GLY	GLU
ILE	ILE	F853	GLY	L707	L707	A555	ARG	ARG	GLY	ARG	GLU
PHE	PHE	L831	ALA	L708	L708	A556	ALA	ALA	GLY	ARG	GLU
CYS	CYS	L831	GLY	M709	M709	A557	PRQ	PRQ	ASP	THR	CYS
GLU	GLU	V942	ALA	K641	K641	R557	ASP	ASP	THR	THR	MET
PHE	PHE	V942	GLY	M642	M642	A561	GLU	GLU	ILE	ALA	GLU
LEU	LEU	T945	GLN	L643	L643	A561	ILE	ILE	ASN	ILE	ILE
ASN	ASN	T945	ILE	H644	H644	H570	PHE	PHE	LYS	ILE	ILE
CYS	CYS	W661	PHE	K649	K649	H570	MET	MET	LYS	ILE	ILE
THR	THR	H862	GLN	W649	W649	V575	GLN	GLN	ILE	PHE	LEU
ARG	ARG	L863	GLN	H719	H719	V575	ALA	ALA	ALA	ALA	ARG
GLY	GLY	L863	LYS	D652	D652	Q579	GLY	GLY	THR	THR	GLY
ILE	ILE	M953	ASN	R653	R653	Q580	ILE	ILE	GLY	GLY	GLU
VAL	VAL	L867	ARG	L723	L723	Q580	LYS	LYS	ARG	ARG	GLU
LEU	LEU	L867	TYR	L726	L726	A581	ALA	ALA	GLY	GLY	GLU
ALA	ALA	L870	PHE	C727	C727	S582	ALA	ALA	SER	SER	HIS
VAL	VAL	L871	MET	L728	L728	F583	THR	THR	PRO	PRO	GLY
LYS	LYS	S873	ASP	W658	W658	L584	LEU	LEU	LEU	LEU	GLY
ALA	ALA	T874	GLY	M659	M659	L584	VAL	VAL	ILE	ILE	TYR
LYS	LYS	W875	ASP	F660	F660	H585	MET	MET	ILE	ILE	SER
THR	THR	W876	S804	K661	K661	H585	ASP	ASP	VAL	VAL	ARG
HIS	HIS	H870	L803	Y662	Y662	K591	GLY	GLY	ALA	ALA	GLN
LYS	LYS	L870	S804	L663	L663	K592	THR	THR	THR	THR	LEU
THR	THR	L871	LYS	L663	L663	K593	ALA	ALA	ALA	ALA	LEU
HIS	HIS	L871	GLY	CYS	CYS	R594	MET	MET	ILE	ILE	HIS
LEU	LEU	L877	ILE	LYS	LYS	E594	ILE	ILE	SER	SER	ILE
PRO	PRO	L878	THR	THR	THR	G505	ALA	ALA	SER	SER	ALA
ALA	ALA	L880	ASN	PRO	PRO	G505	THR	THR	TYR	TYR	ALA
VAL	VAL	L881	LYS	GLU	GLU	H512	ASN	ASN	SER	SER	PRO
LYS	LYS	L882	ILE	PHE	PHE	H512	PRO	PRO	ILE	ILE	THR
THR	THR	L882	THR	THR	THR	H512	LEU	LEU	VAL	VAL	PRO
HIS	HIS	L885	THR	THR	THR	H512	ASN	ASN	LEU	LEU	LEU
LYS	LYS	L886	THR	THR	THR	H512	GLY	GLY	VAL	VAL	GLY
THR	THR	L886	THR	THR	THR	H512	THR	THR	THR	THR	THR
ALA	ALA	L889	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
VAL	VAL	L890	THR	THR	THR	H512	LEU	LEU	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	VAL	VAL	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	ALA	ALA	THR	THR	THR
ALA	ALA	L891	THR	THR	THR	H512	LEU	LEU	THR	THR	THR
VAL	VAL	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
ALA	ALA	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
VAL	VAL	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
ALA	ALA	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
VAL	VAL	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
HIS	HIS	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
ALA	ALA	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
VAL	VAL	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
HIS	HIS	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
ALA	ALA	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
VAL	VAL	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
HIS	HIS	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
ALA	ALA	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
VAL	VAL	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
HIS	HIS	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
ALA	ALA	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
VAL	VAL	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
HIS	HIS	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
ALA	ALA	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
VAL	VAL	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
HIS	HIS	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
ALA	ALA	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
VAL	VAL	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
HIS	HIS	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
ALA	ALA	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
VAL	VAL	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
HIS	HIS	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
ALA	ALA	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
VAL	VAL	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
HIS	HIS	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
ALA	ALA	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
VAL	VAL	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
HIS	HIS	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
ALA	ALA	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
VAL	VAL	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
HIS	HIS	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
ALA	ALA	L891	THR	THR	THR	H512	ASN	ASN	THR	THR	THR
VAL	VAL	L891	THR	THR	THR	H512	GLY	GLY	THR	THR	THR
LYS	LYS	L891	THR	THR	THR	H512	THR	THR	THR	THR	THR
THR	THR	L891	THR	THR	THR	H512	ASN	ASN			

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	43585	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI Polara 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	21	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	31000	Depositor
Image detector	Gatan K2 (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	0.41	0/4326	0.82	1/5872 (0.0%)
1	B	0.41	0/4326	0.82	1/5872 (0.0%)
1	C	0.42	0/4326	0.82	1/5872 (0.0%)
1	D	0.41	0/4326	0.82	1/5872 (0.0%)
All	All	0.41	0/17304	0.82	4/23488 (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	0	23
1	B	0	23
1	C	0	23
1	D	0	24
All	All	0	93

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	766	ASN	N-CA-CB	9.05	126.89	110.60
1	D	766	ASN	N-CA-CB	9.02	126.84	110.60
1	C	766	ASN	N-CA-CB	9.02	126.84	110.60
1	B	766	ASN	N-CA-CB	9.00	126.80	110.60

There are no chirality outliers.

All (93) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1032	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	1047	GLN	Sidechain
1	A	547	ASP	Peptide
1	A	593	LYS	Peptide
1	A	604	ARG	Peptide
1	A	609	LEU	Peptide
1	A	610	LYS	Peptide
1	A	612	PHE	Peptide
1	A	626	MET	Peptide
1	A	643	LEU	Peptide
1	A	644	HIS	Peptide
1	A	682	PRO	Peptide
1	A	692	ASN	Peptide
1	A	693	ASN	Peptide
1	A	695	ILE	Peptide
1	A	696	GLU	Peptide
1	A	740	ILE	Peptide
1	A	745	ALA	Peptide
1	A	826	ILE	Peptide
1	A	893	ASN	Peptide
1	A	897	PRO	Peptide
1	A	913	LEU	Peptide
1	A	918	TYR	Peptide
1	B	1032	GLU	Peptide
1	B	1047	GLN	Sidechain
1	B	547	ASP	Peptide
1	B	593	LYS	Peptide
1	B	604	ARG	Peptide
1	B	609	LEU	Peptide
1	B	610	LYS	Peptide
1	B	612	PHE	Peptide
1	B	626	MET	Peptide
1	B	643	LEU	Peptide
1	B	644	HIS	Peptide
1	B	682	PRO	Peptide
1	B	692	ASN	Peptide
1	B	693	ASN	Peptide
1	B	695	ILE	Peptide
1	B	696	GLU	Peptide
1	B	740	ILE	Peptide
1	B	745	ALA	Peptide
1	B	826	ILE	Peptide
1	B	893	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	B	897	PRO	Peptide
1	B	913	LEU	Peptide
1	B	918	TYR	Peptide
1	C	1032	GLU	Peptide
1	C	1047	GLN	Sidechain
1	C	547	ASP	Peptide
1	C	593	LYS	Peptide
1	C	604	ARG	Peptide
1	C	609	LEU	Peptide
1	C	610	LYS	Peptide
1	C	612	PHE	Peptide
1	C	626	MET	Peptide
1	C	643	LEU	Peptide
1	C	644	HIS	Peptide
1	C	682	PRO	Peptide
1	C	692	ASN	Peptide
1	C	693	ASN	Peptide
1	C	695	ILE	Peptide
1	C	696	GLU	Peptide
1	C	740	ILE	Peptide
1	C	745	ALA	Peptide
1	C	826	ILE	Peptide
1	C	893	ASN	Peptide
1	C	897	PRO	Peptide
1	C	913	LEU	Peptide
1	C	918	TYR	Peptide
1	D	1032	GLU	Peptide
1	D	1047	GLN	Sidechain
1	D	547	ASP	Peptide
1	D	593	LYS	Peptide
1	D	604	ARG	Peptide
1	D	609	LEU	Peptide
1	D	610	LYS	Peptide
1	D	612	PHE	Peptide
1	D	626	MET	Peptide
1	D	643	LEU	Peptide
1	D	644	HIS	Peptide
1	D	682	PRO	Peptide
1	D	692	ASN	Peptide
1	D	693	ASN	Peptide
1	D	695	ILE	Peptide
1	D	696	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	D	740	ILE	Peptide
1	D	745	ALA	Peptide
1	D	826	ILE	Peptide
1	D	893	ASN	Peptide
1	D	897	PRO	Peptide
1	D	913	LEU	Peptide
1	D	917	ASN	Peptide
1	D	918	TYR	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	4238	0	4110	232	0
1	B	4238	0	4110	230	0
1	C	4238	0	4110	233	0
1	D	4238	0	4110	239	0
All	All	16952	0	16440	851	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 25.

All (851) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1051:LEU:HD13	1:A:1047:GLN:NE2	1.39	1.37
1:A:1051:LEU:HD13	1:B:1047:GLN:NE2	1.40	1.32
1:B:1051:LEU:HD13	1:C:1047:GLN:NE2	1.41	1.32
1:D:1047:GLN:NE2	1:C:1051:LEU:HD13	1.40	1.30
1:D:1051:LEU:CD1	1:A:1047:GLN:NE2	2.26	0.97
1:A:1051:LEU:CD1	1:B:1047:GLN:NE2	2.27	0.96
1:D:1047:GLN:NE2	1:C:1051:LEU:CD1	2.27	0.96
1:D:1051:LEU:HD13	1:A:1047:GLN:HE22	1.14	0.95
1:B:1051:LEU:CD1	1:C:1047:GLN:NE2	2.29	0.95
1:B:1051:LEU:HD13	1:C:1047:GLN:HE22	1.17	0.94
1:D:1047:GLN:HE22	1:C:1051:LEU:HD13	1.14	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1051:LEU:HD13	1:B:1047:GLN:HE22	1.16	0.93
1:B:629:TYR:H	1:B:697:LEU:HD11	1.41	0.86
1:A:629:TYR:H	1:A:697:LEU:HD11	1.41	0.85
1:D:629:TYR:H	1:D:697:LEU:HD11	1.41	0.84
1:A:1072:MET:O	1:B:458:ARG:NH2	2.11	0.83
1:C:629:TYR:H	1:C:697:LEU:HD11	1.41	0.83
1:A:970:HIS:ND1	1:A:970:HIS:O	2.12	0.82
1:D:970:HIS:ND1	1:D:970:HIS:O	2.12	0.82
1:D:540:CYS:HA	1:D:543:ARG:HH21	1.44	0.82
1:A:540:CYS:HA	1:A:543:ARG:HH21	1.44	0.82
1:B:540:CYS:HA	1:B:543:ARG:HH21	1.44	0.82
1:B:1072:MET:O	1:C:458:ARG:NH2	2.12	0.81
1:D:1072:MET:O	1:A:458:ARG:NH2	2.13	0.81
1:C:970:HIS:ND1	1:C:970:HIS:O	2.12	0.81
1:C:540:CYS:HA	1:C:543:ARG:HH21	1.44	0.81
1:D:458:ARG:NH2	1:C:1072:MET:O	2.14	0.81
1:B:970:HIS:O	1:B:970:HIS:ND1	2.12	0.80
1:D:1051:LEU:HD13	1:A:1047:GLN:HE21	1.46	0.80
1:A:1051:LEU:HD13	1:B:1047:GLN:HE21	1.47	0.79
1:B:1051:LEU:HD13	1:C:1047:GLN:HE21	1.48	0.78
1:D:1047:GLN:HE21	1:C:1051:LEU:HD13	1.49	0.78
1:B:925:PRO:HB2	1:B:931:LEU:HD23	1.66	0.78
1:B:811:ILE:HD11	1:B:842:TYR:CD1	2.19	0.77
1:D:925:PRO:HB2	1:D:931:LEU:HD23	1.66	0.77
1:B:1051:LEU:CD1	1:C:1047:GLN:HE22	1.96	0.77
1:A:811:ILE:HD11	1:A:842:TYR:CD1	2.19	0.77
1:C:811:ILE:HD11	1:C:842:TYR:CD1	2.19	0.77
1:D:811:ILE:HD11	1:D:842:TYR:CD1	2.19	0.77
1:C:925:PRO:HB2	1:C:931:LEU:HD23	1.65	0.77
1:D:695:ILE:HD13	1:D:698:LEU:HB3	1.67	0.76
1:A:925:PRO:HB2	1:A:931:LEU:HD23	1.66	0.76
1:D:579:GLN:O	1:D:581:ALA:N	2.18	0.76
1:B:695:ILE:HD13	1:B:698:LEU:HB3	1.67	0.76
1:A:695:ILE:HD13	1:A:698:LEU:HB3	1.67	0.76
1:A:1051:LEU:CD1	1:B:1047:GLN:HE22	1.95	0.75
1:C:579:GLN:O	1:C:581:ALA:N	2.18	0.75
1:A:631:PRO:O	1:A:634:MET:N	2.20	0.75
1:D:631:PRO:O	1:D:634:MET:N	2.20	0.75
1:B:579:GLN:O	1:B:581:ALA:N	2.18	0.75
1:D:540:CYS:HA	1:D:543:ARG:NH2	2.01	0.75
1:B:882:LEU:HA	1:B:905:ILE:HD13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:631:PRO:O	1:C:634:MET:N	2.20	0.75
1:B:631:PRO:O	1:B:634:MET:N	2.20	0.75
1:C:540:CYS:HA	1:C:543:ARG:NH2	2.01	0.75
1:C:882:LEU:HA	1:C:905:ILE:HD13	1.68	0.75
1:C:695:ILE:HD13	1:C:698:LEU:HB3	1.67	0.74
1:A:540:CYS:HA	1:A:543:ARG:NH2	2.01	0.74
1:B:540:CYS:HA	1:B:543:ARG:NH2	2.01	0.74
1:A:579:GLN:O	1:A:581:ALA:N	2.18	0.74
1:A:882:LEU:HA	1:A:905:ILE:HD13	1.68	0.73
1:D:1000:GLN:OE1	1:D:1000:GLN:N	2.21	0.73
1:D:1065:ILE:HA	1:D:1068:ILE:HG12	1.71	0.73
1:C:1000:GLN:OE1	1:C:1000:GLN:N	2.21	0.73
1:D:591:LYS:HA	1:D:627:ILE:HD11	1.70	0.73
1:D:882:LEU:HA	1:D:905:ILE:HD13	1.68	0.73
1:B:591:LYS:HA	1:B:627:ILE:HD11	1.70	0.73
1:A:1065:ILE:HA	1:A:1068:ILE:HG12	1.71	0.73
1:A:832:TRP:HA	1:A:832:TRP:CE3	2.24	0.73
1:C:832:TRP:HA	1:C:832:TRP:CE3	2.24	0.72
1:A:1000:GLN:N	1:A:1000:GLN:OE1	2.21	0.72
1:B:1000:GLN:N	1:B:1000:GLN:OE1	2.21	0.72
1:B:522:SER:HB3	1:B:555:ALA:HB2	1.71	0.72
1:B:832:TRP:HA	1:B:832:TRP:CE3	2.24	0.72
1:C:1065:ILE:HA	1:C:1068:ILE:HG12	1.71	0.72
1:D:832:TRP:CE3	1:D:832:TRP:HA	2.24	0.71
1:D:1051:LEU:CD1	1:A:1047:GLN:HE22	1.94	0.71
1:C:832:TRP:HA	1:C:832:TRP:HE3	1.55	0.71
1:B:832:TRP:HA	1:B:832:TRP:HE3	1.56	0.71
1:A:591:LYS:HA	1:A:627:ILE:HD11	1.70	0.71
1:C:522:SER:HB3	1:C:555:ALA:HB2	1.71	0.71
1:B:1065:ILE:HA	1:B:1068:ILE:HG12	1.71	0.71
1:C:591:LYS:HA	1:C:627:ILE:HD11	1.70	0.71
1:B:885:GLY:HA2	1:B:908:THR:HG21	1.73	0.71
1:A:885:GLY:HA2	1:A:908:THR:HG21	1.73	0.71
1:D:1047:GLN:HE22	1:C:1051:LEU:CD1	1.94	0.71
1:D:885:GLY:HA2	1:D:908:THR:HG21	1.73	0.71
1:A:522:SER:HB3	1:A:555:ALA:HB2	1.71	0.70
1:A:832:TRP:HA	1:A:832:TRP:HE3	1.55	0.70
1:D:832:TRP:HE3	1:D:832:TRP:HA	1.55	0.70
1:D:468:ASP:H	1:D:469:ILE:HA	1.56	0.70
1:B:468:ASP:H	1:B:469:ILE:HA	1.56	0.70
1:C:468:ASP:H	1:C:469:ILE:HA	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ASP:H	1:A:469:ILE:HA	1.56	0.70
1:D:522:SER:HB3	1:D:555:ALA:HB2	1.71	0.69
1:C:638:LEU:HD11	1:C:653:ASP:HB2	1.75	0.69
1:B:638:LEU:HD11	1:B:653:ASP:HB2	1.75	0.69
1:C:885:GLY:HA2	1:C:908:THR:HG21	1.73	0.69
1:B:545:ASP:HB3	1:B:546:GLU:HA	1.75	0.69
1:B:631:PRO:HB2	1:B:697:LEU:HD22	1.76	0.68
1:D:638:LEU:HD11	1:D:653:ASP:HB2	1.75	0.68
1:C:545:ASP:HB3	1:C:546:GLU:HA	1.75	0.68
1:D:544:LEU:O	1:D:548:GLY:HA2	1.94	0.68
1:A:544:LEU:O	1:A:548:GLY:HA2	1.93	0.68
1:A:638:LEU:HD11	1:A:653:ASP:HB2	1.75	0.68
1:D:545:ASP:HB3	1:D:546:GLU:HA	1.75	0.68
1:B:516:THR:HG22	1:B:517:ALA:H	1.58	0.68
1:B:542:ASP:O	1:B:543:ARG:HD3	1.94	0.68
1:C:542:ASP:O	1:C:543:ARG:HD3	1.94	0.68
1:C:516:THR:HG22	1:C:517:ALA:H	1.58	0.68
1:A:743:GLY:H	1:A:832:TRP:HE1	1.42	0.67
1:B:544:LEU:O	1:B:548:GLY:HA2	1.93	0.67
1:C:631:PRO:HB2	1:C:697:LEU:HD22	1.75	0.67
1:A:631:PRO:HB2	1:A:697:LEU:HD22	1.76	0.67
1:D:542:ASP:O	1:D:543:ARG:HD3	1.94	0.67
1:D:516:THR:HG22	1:D:517:ALA:H	1.58	0.67
1:C:544:LEU:O	1:C:548:GLY:HA2	1.93	0.67
1:A:516:THR:HG22	1:A:517:ALA:H	1.58	0.67
1:C:743:GLY:H	1:C:832:TRP:HE1	1.43	0.67
1:D:631:PRO:HB2	1:D:697:LEU:HD22	1.75	0.67
1:B:743:GLY:H	1:B:832:TRP:HE1	1.43	0.66
1:A:542:ASP:O	1:A:543:ARG:HD3	1.94	0.66
1:A:545:ASP:HB3	1:A:546:GLU:HA	1.75	0.66
1:D:743:GLY:H	1:D:832:TRP:HE1	1.42	0.66
1:B:515:TRP:O	1:B:519:HIS:ND1	2.29	0.66
1:D:804:SER:HA	1:D:807:LEU:HD12	1.78	0.66
1:C:515:TRP:O	1:C:519:HIS:ND1	2.29	0.66
1:C:804:SER:HA	1:C:807:LEU:HD12	1.78	0.66
1:A:992:LEU:HA	1:A:995:LEU:HD23	1.78	0.65
1:A:1069:ILE:HD11	1:B:1064:LEU:HD21	1.78	0.65
1:B:992:LEU:HA	1:B:995:LEU:HD23	1.78	0.65
1:A:804:SER:HA	1:A:807:LEU:HD12	1.78	0.65
1:A:515:TRP:O	1:A:519:HIS:ND1	2.29	0.65
1:B:804:SER:HA	1:B:807:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1064:LEU:HD21	1:C:1069:ILE:HD11	1.79	0.65
1:D:561:ALA:HB1	1:D:598:THR:HG21	1.80	0.64
1:B:1069:ILE:HD11	1:C:1064:LEU:HD21	1.78	0.64
1:D:1069:ILE:HD11	1:A:1064:LEU:HD21	1.79	0.64
1:D:515:TRP:O	1:D:519:HIS:ND1	2.29	0.64
1:D:992:LEU:HA	1:D:995:LEU:HD23	1.78	0.64
1:C:561:ALA:HB1	1:C:598:THR:HG21	1.79	0.64
1:A:561:ALA:HB1	1:A:598:THR:HG21	1.79	0.64
1:B:640:PHE:HD2	1:B:642:MET:HB3	1.63	0.63
1:A:640:PHE:HD2	1:A:642:MET:HB3	1.63	0.63
1:C:992:LEU:HA	1:C:995:LEU:HD23	1.78	0.63
1:B:561:ALA:HB1	1:B:598:THR:HG21	1.80	0.63
1:B:496:LYS:NZ	1:B:496:LYS:HA	2.15	0.62
1:C:871:LEU:O	1:C:874:THR:HG22	2.00	0.62
1:D:640:PHE:HD2	1:D:642:MET:HB3	1.63	0.62
1:D:1048:LYS:HZ3	1:A:1050:ARG:NH2	1.97	0.62
1:D:889:TYR:O	1:D:893:ASN:ND2	2.33	0.62
1:A:496:LYS:NZ	1:A:496:LYS:HA	2.15	0.62
1:C:640:PHE:HD2	1:C:642:MET:HB3	1.62	0.62
1:C:496:LYS:HA	1:C:496:LYS:NZ	2.14	0.62
1:B:811:ILE:HD11	1:B:842:TYR:HD1	1.64	0.62
1:A:889:TYR:O	1:A:893:ASN:ND2	2.33	0.62
1:D:496:LYS:HA	1:D:496:LYS:NZ	2.15	0.62
1:B:889:TYR:O	1:B:893:ASN:ND2	2.33	0.61
1:C:889:TYR:O	1:C:893:ASN:ND2	2.33	0.61
1:B:582:SER:O	1:B:585:HIS:HB2	2.00	0.61
1:A:923:LEU:HD22	1:B:897:PRO:HG3	1.82	0.61
1:D:871:LEU:O	1:D:874:THR:HG22	2.00	0.61
1:A:582:SER:O	1:A:585:HIS:HB2	2.00	0.61
1:D:917:ASN:H	1:D:918:TYR:CB	2.13	0.61
1:B:871:LEU:O	1:B:874:THR:HG22	2.00	0.61
1:D:875:VAL:O	1:D:878:ILE:HG22	2.01	0.61
1:B:997:LYS:HB2	1:B:998:VAL:HA	1.83	0.61
1:C:917:ASN:H	1:C:918:TYR:CB	2.13	0.61
1:B:875:VAL:O	1:B:878:ILE:HG22	2.01	0.61
1:A:871:LEU:O	1:A:874:THR:HG22	2.00	0.61
1:A:875:VAL:O	1:A:878:ILE:HG22	2.01	0.61
1:A:917:ASN:H	1:A:918:TYR:CB	2.13	0.61
1:A:811:ILE:HD11	1:A:842:TYR:HD1	1.64	0.60
1:C:997:LYS:HB2	1:C:998:VAL:HA	1.83	0.60
1:C:875:VAL:O	1:C:878:ILE:HG22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:877:PHE:HA	1:D:880:LEU:HB3	1.82	0.60
1:A:997:LYS:HB2	1:A:998:VAL:HA	1.83	0.60
1:A:553:HIS:CE1	1:A:583:PHE:HB3	2.37	0.60
1:C:582:SER:O	1:C:585:HIS:HB2	2.00	0.60
1:D:811:ILE:HD11	1:D:842:TYR:HD1	1.64	0.60
1:B:923:LEU:HD22	1:C:897:PRO:HG3	1.83	0.60
1:C:877:PHE:HA	1:C:880:LEU:HB3	1.82	0.60
1:B:917:ASN:H	1:B:918:TYR:CB	2.13	0.60
1:D:582:SER:O	1:D:585:HIS:HB2	2.00	0.60
1:C:660:PHE:HB3	1:C:661:LYS:C	2.22	0.60
1:A:1048:LYS:HZ3	1:B:1050:ARG:NH2	2.00	0.60
1:B:877:PHE:HA	1:B:880:LEU:HB3	1.82	0.60
1:A:877:PHE:HA	1:A:880:LEU:HB3	1.82	0.60
1:C:553:HIS:CE1	1:C:583:PHE:HB3	2.37	0.60
1:D:660:PHE:HB3	1:D:661:LYS:C	2.23	0.60
1:B:553:HIS:CE1	1:B:583:PHE:HB3	2.36	0.59
1:C:809:TRP:O	1:C:813:THR:HG23	2.02	0.59
1:D:1050:ARG:NH2	1:C:1048:LYS:HZ3	2.00	0.59
1:D:997:LYS:HB2	1:D:998:VAL:HA	1.83	0.59
1:B:660:PHE:HB3	1:B:661:LYS:C	2.22	0.59
1:A:916:ILE:N	1:A:917:ASN:HA	2.18	0.59
1:A:891:LEU:HB3	1:A:892:LEU:HD22	1.85	0.59
1:A:990:LEU:HD11	1:A:994:PHE:HD2	1.68	0.59
1:B:809:TRP:O	1:B:813:THR:HG23	2.02	0.59
1:D:891:LEU:HB3	1:D:892:LEU:HD22	1.85	0.59
1:D:766:ASN:OD1	1:D:769:LEU:CB	2.51	0.59
1:A:766:ASN:OD1	1:A:769:LEU:CB	2.51	0.59
1:D:818:PHE:HD2	1:D:835:GLY:HA2	1.67	0.59
1:D:916:ILE:N	1:D:917:ASN:HA	2.18	0.59
1:D:809:TRP:O	1:D:813:THR:HG23	2.02	0.59
1:A:660:PHE:HB3	1:A:661:LYS:C	2.22	0.59
1:B:766:ASN:OD1	1:B:769:LEU:CB	2.51	0.59
1:D:553:HIS:CE1	1:D:583:PHE:HB3	2.37	0.59
1:B:818:PHE:HD2	1:B:835:GLY:HA2	1.67	0.58
1:A:824:VAL:HG12	1:A:825:GLU:N	2.18	0.58
1:C:891:LEU:HB3	1:C:892:LEU:HD22	1.85	0.58
1:B:891:LEU:HB3	1:B:892:LEU:HD22	1.85	0.58
1:B:824:VAL:HG12	1:B:825:GLU:N	2.18	0.58
1:D:990:LEU:HD11	1:D:994:PHE:HD2	1.68	0.58
1:A:990:LEU:HD11	1:A:994:PHE:CD2	2.39	0.58
1:B:990:LEU:HD11	1:B:994:PHE:CD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:990:LEU:HD11	1:B:994:PHE:HD2	1.68	0.58
1:D:824:VAL:HG12	1:D:825:GLU:N	2.18	0.58
1:A:809:TRP:O	1:A:813:THR:HG23	2.02	0.58
1:C:455:SER:HA	1:C:488:LEU:HB3	1.86	0.58
1:D:990:LEU:HD11	1:D:994:PHE:CD2	2.39	0.58
1:D:923:LEU:HD22	1:A:897:PRO:HG3	1.85	0.58
1:D:455:SER:HA	1:D:488:LEU:HB3	1.86	0.58
1:C:990:LEU:HD11	1:C:994:PHE:CD2	2.39	0.58
1:C:766:ASN:OD1	1:C:769:LEU:CB	2.51	0.58
1:B:452:PHE:CE1	1:B:1071:LYS:HE3	2.39	0.58
1:C:990:LEU:HD11	1:C:994:PHE:HD2	1.68	0.58
1:C:968:GLN:HA	1:C:971:ALA:HB2	1.85	0.58
1:A:686:LEU:HD22	1:A:708:LEU:HD11	1.86	0.58
1:C:824:VAL:HG12	1:C:825:GLU:N	2.18	0.58
1:B:1048:LYS:HZ3	1:C:1050:ARG:NH2	2.02	0.57
1:C:818:PHE:HD2	1:C:835:GLY:HA2	1.67	0.57
1:A:818:PHE:HD2	1:A:835:GLY:HA2	1.68	0.57
1:C:916:ILE:N	1:C:917:ASN:HA	2.18	0.57
1:D:686:LEU:HD22	1:D:708:LEU:HD11	1.86	0.57
1:B:916:ILE:N	1:B:917:ASN:HA	2.18	0.57
1:B:851:GLN:O	1:B:857:GLY:HA2	2.05	0.57
1:B:968:GLN:HA	1:B:971:ALA:HB2	1.85	0.57
1:A:851:GLN:O	1:A:857:GLY:HA2	2.05	0.57
1:C:452:PHE:CE1	1:C:1071:LYS:HE3	2.39	0.57
1:D:452:PHE:CE1	1:D:1071:LYS:HE3	2.39	0.57
1:B:455:SER:HA	1:B:488:LEU:HB3	1.86	0.57
1:C:480:LEU:HD12	1:C:481:HIS:HA	1.87	0.57
1:A:968:GLN:HA	1:A:971:ALA:HB2	1.85	0.57
1:B:686:LEU:HD22	1:B:708:LEU:HD11	1.86	0.57
1:B:480:LEU:HD12	1:B:481:HIS:HA	1.87	0.57
1:C:811:ILE:HD11	1:C:842:TYR:HD1	1.65	0.56
1:D:851:GLN:O	1:D:857:GLY:HA2	2.05	0.56
1:C:686:LEU:HD22	1:C:708:LEU:HD11	1.86	0.56
1:A:452:PHE:CE1	1:A:1071:LYS:HE3	2.39	0.56
1:A:480:LEU:HD12	1:A:481:HIS:HA	1.87	0.56
1:D:480:LEU:HD12	1:D:481:HIS:HA	1.87	0.56
1:D:968:GLN:HA	1:D:971:ALA:HB2	1.85	0.56
1:C:851:GLN:O	1:C:857:GLY:HA2	2.05	0.56
1:A:455:SER:HA	1:A:488:LEU:HB3	1.86	0.56
1:B:698:LEU:HD21	1:B:976:ILE:HG21	1.88	0.55
1:D:456:TYR:O	1:D:494:HIS:NE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:TYR:O	1:B:494:HIS:NE2	2.40	0.55
1:D:897:PRO:HG3	1:C:923:LEU:HD22	1.87	0.55
1:C:945:THR:HA	1:C:949:PRO:HD2	1.88	0.55
1:C:456:TYR:O	1:C:494:HIS:NE2	2.40	0.55
1:C:698:LEU:HD21	1:C:976:ILE:HG21	1.87	0.55
1:A:455:SER:HB2	1:A:488:LEU:HD23	1.89	0.55
1:C:480:LEU:HA	1:C:481:HIS:C	2.27	0.55
1:A:575:VAL:HA	1:A:610:LYS:HE3	1.88	0.55
1:A:698:LEU:HD21	1:A:976:ILE:HG21	1.87	0.55
1:D:698:LEU:HD21	1:D:976:ILE:HG21	1.88	0.55
1:D:945:THR:HA	1:D:949:PRO:HD2	1.88	0.55
1:A:687:ASN:O	1:A:690:VAL:HG12	2.07	0.55
1:A:480:LEU:HA	1:A:481:HIS:C	2.27	0.55
1:A:945:THR:HA	1:A:949:PRO:HD2	1.88	0.55
1:C:575:VAL:HA	1:C:610:LYS:HE3	1.88	0.55
1:B:945:THR:HA	1:B:949:PRO:HD2	1.88	0.55
1:A:870:LEU:CD2	1:A:956:LEU:HD11	2.38	0.55
1:D:687:ASN:O	1:D:690:VAL:HG12	2.07	0.54
1:D:1047:GLN:HE21	1:C:1051:LEU:CD1	2.13	0.54
1:A:456:TYR:O	1:A:494:HIS:NE2	2.39	0.54
1:A:876:VAL:HG11	1:B:859:PHE:CD2	2.42	0.54
1:B:455:SER:HB2	1:B:488:LEU:HD23	1.89	0.54
1:B:575:VAL:HA	1:B:610:LYS:HE3	1.88	0.54
1:B:870:LEU:CD2	1:B:956:LEU:HD11	2.37	0.54
1:B:876:VAL:HG11	1:C:859:PHE:CD2	2.42	0.54
1:B:687:ASN:O	1:B:690:VAL:HG12	2.07	0.54
1:D:580:GLN:HG2	1:D:581:ALA:N	2.23	0.54
1:D:480:LEU:HA	1:D:481:HIS:C	2.27	0.54
1:C:455:SER:HB2	1:C:488:LEU:HD23	1.89	0.54
1:B:480:LEU:HA	1:B:481:HIS:C	2.27	0.54
1:D:870:LEU:CD2	1:D:956:LEU:HD11	2.37	0.54
1:D:848:LEU:O	1:D:851:GLN:HB3	2.08	0.54
1:C:687:ASN:O	1:C:690:VAL:HG12	2.07	0.54
1:B:1051:LEU:CD1	1:C:1047:GLN:HE21	2.13	0.54
1:B:848:LEU:O	1:B:851:GLN:HB3	2.08	0.54
1:D:575:VAL:HA	1:D:610:LYS:HE3	1.88	0.54
1:D:455:SER:HB2	1:D:488:LEU:HD23	1.89	0.53
1:A:580:GLN:HG2	1:A:581:ALA:N	2.23	0.53
1:B:918:TYR:HD1	1:B:921:SER:HB3	1.74	0.53
1:A:848:LEU:O	1:A:851:GLN:HB3	2.08	0.53
1:B:977:ALA:HA	1:B:980:VAL:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:GLN:HG2	1:B:581:ALA:N	2.23	0.53
1:A:977:ALA:HA	1:A:980:VAL:HG12	1.91	0.53
1:C:977:ALA:HA	1:C:980:VAL:HG12	1.91	0.53
1:C:870:LEU:CD2	1:C:956:LEU:HD11	2.37	0.53
1:A:597:LEU:CD1	1:A:601:ARG:HH12	2.22	0.53
1:D:597:LEU:CD1	1:D:601:ARG:HH12	2.22	0.53
1:A:1047:GLN:HA	1:A:1050:ARG:HH21	1.74	0.53
1:C:710:LYS:O	1:C:713:ALA:N	2.41	0.53
1:D:518:LEU:HD12	1:D:521:ALA:HB3	1.91	0.53
1:D:876:VAL:HG11	1:A:859:PHE:CD2	2.44	0.53
1:C:580:GLN:HG2	1:C:581:ALA:N	2.23	0.53
1:B:619:ASN:O	1:B:622:PRO:HD2	2.09	0.53
1:A:918:TYR:HD1	1:A:921:SER:HB3	1.74	0.52
1:D:710:LYS:O	1:D:713:ALA:N	2.40	0.52
1:B:874:THR:HA	1:B:877:PHE:CZ	2.44	0.52
1:C:918:TYR:HD1	1:C:921:SER:HB3	1.74	0.52
1:A:917:ASN:H	1:A:918:TYR:HB2	1.74	0.52
1:D:977:ALA:HA	1:D:980:VAL:HG12	1.91	0.52
1:C:1047:GLN:HA	1:C:1050:ARG:HH21	1.74	0.52
1:C:874:THR:HA	1:C:877:PHE:CZ	2.44	0.52
1:A:923:LEU:HD11	1:B:897:PRO:HB3	1.91	0.52
1:B:609:LEU:HB2	1:B:610:LYS:HG3	1.92	0.52
1:A:619:ASN:O	1:A:622:PRO:HD2	2.09	0.52
1:D:619:ASN:O	1:D:622:PRO:HD2	2.09	0.52
1:B:597:LEU:CD1	1:B:601:ARG:HH12	2.22	0.52
1:C:917:ASN:H	1:C:918:TYR:HB2	1.73	0.52
1:B:824:VAL:HG12	1:B:825:GLU:H	1.75	0.52
1:D:859:PHE:O	1:D:862:MET:HB3	2.10	0.52
1:D:874:THR:HA	1:D:877:PHE:CZ	2.44	0.52
1:D:918:TYR:HD1	1:D:921:SER:HB3	1.74	0.52
1:C:859:PHE:O	1:C:862:MET:HB3	2.10	0.52
1:C:848:LEU:O	1:C:851:GLN:HB3	2.08	0.52
1:B:518:LEU:HD12	1:B:521:ALA:HB3	1.91	0.52
1:D:1047:GLN:HA	1:D:1050:ARG:HH21	1.74	0.52
1:D:917:ASN:H	1:D:918:TYR:HB2	1.74	0.52
1:B:917:ASN:H	1:B:918:TYR:HB2	1.74	0.52
1:D:859:PHE:CD2	1:C:876:VAL:HG11	2.44	0.52
1:A:874:THR:HA	1:A:877:PHE:CZ	2.44	0.52
1:A:859:PHE:O	1:A:862:MET:HB3	2.10	0.52
1:D:824:VAL:HG12	1:D:825:GLU:H	1.75	0.52
1:A:1061:GLN:NE2	1:B:1061:GLN:HE22	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LYS:HG3	1:A:492:ASN:OD1	2.11	0.52
1:B:1047:GLN:HA	1:B:1050:ARG:HH21	1.74	0.51
1:A:518:LEU:HD12	1:A:521:ALA:HB3	1.91	0.51
1:B:491:LYS:HG3	1:B:492:ASN:OD1	2.11	0.51
1:A:885:GLY:O	1:A:904:SER:OG	2.28	0.51
1:D:1061:GLN:NE2	1:A:1061:GLN:HE22	2.08	0.51
1:C:597:LEU:CD1	1:C:601:ARG:HH12	2.22	0.51
1:C:619:ASN:O	1:C:622:PRO:HD2	2.09	0.51
1:D:609:LEU:HB2	1:D:610:LYS:HG3	1.92	0.51
1:D:726:TYR:HE2	1:D:846:PHE:HB2	1.76	0.51
1:C:518:LEU:HD12	1:C:521:ALA:HB3	1.91	0.51
1:D:885:GLY:O	1:D:904:SER:OG	2.28	0.51
1:A:824:VAL:HG12	1:A:825:GLU:H	1.75	0.51
1:C:824:VAL:HG12	1:C:825:GLU:H	1.75	0.51
1:C:609:LEU:HB2	1:C:610:LYS:HG3	1.92	0.51
1:C:726:TYR:HE2	1:C:846:PHE:HB2	1.76	0.51
1:B:859:PHE:O	1:B:862:MET:HB3	2.10	0.51
1:B:1061:GLN:NE2	1:C:1061:GLN:HE22	2.09	0.51
1:C:885:GLY:O	1:C:904:SER:OG	2.29	0.51
1:A:620:LYS:O	1:A:623:ILE:HB	2.11	0.51
1:B:885:GLY:O	1:B:904:SER:OG	2.29	0.50
1:A:609:LEU:HB2	1:A:610:LYS:HG3	1.92	0.50
1:C:491:LYS:HG3	1:C:492:ASN:OD1	2.10	0.50
1:B:923:LEU:HD11	1:C:897:PRO:HB3	1.92	0.50
1:D:491:LYS:HG3	1:D:492:ASN:OD1	2.11	0.50
1:B:710:LYS:O	1:B:713:ALA:N	2.41	0.50
1:D:897:PRO:HB3	1:C:923:LEU:HD11	1.94	0.50
1:C:773:CYS:O	1:C:777:VAL:HG23	2.12	0.50
1:D:773:CYS:O	1:D:777:VAL:HG23	2.12	0.50
1:A:710:LYS:O	1:A:713:ALA:N	2.40	0.50
1:B:620:LYS:O	1:B:623:ILE:HB	2.11	0.50
1:D:723:LEU:HD23	1:D:727:CYS:HB2	1.94	0.50
1:D:620:LYS:O	1:D:623:ILE:HB	2.11	0.50
1:A:1048:LYS:HZ1	1:B:1050:ARG:HH12	1.60	0.50
1:A:726:TYR:HE2	1:A:846:PHE:HB2	1.76	0.50
1:A:723:LEU:HD23	1:A:727:CYS:HB2	1.94	0.50
1:B:773:CYS:O	1:B:777:VAL:HG23	2.12	0.50
1:B:1048:LYS:HZ1	1:C:1050:ARG:HH12	1.58	0.49
1:B:723:LEU:HD23	1:B:727:CYS:HB2	1.94	0.49
1:C:620:LYS:O	1:C:623:ILE:HB	2.11	0.49
1:C:723:LEU:HD23	1:C:727:CYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1047:GLN:HA	1:B:1050:ARG:NH2	2.28	0.49
1:A:981:GLU:O	1:A:984:THR:HG22	2.13	0.49
1:C:872:ARG:O	1:C:875:VAL:HG12	2.13	0.49
1:B:726:TYR:HE2	1:B:846:PHE:HB2	1.76	0.49
1:D:918:TYR:CD1	1:D:921:SER:HB3	2.47	0.49
1:A:773:CYS:O	1:A:777:VAL:HG23	2.12	0.49
1:C:1047:GLN:HA	1:C:1050:ARG:NH2	2.28	0.49
1:D:496:LYS:HA	1:D:496:LYS:HZ2	1.75	0.49
1:D:981:GLU:O	1:D:984:THR:HG22	2.12	0.49
1:C:918:TYR:CD1	1:C:921:SER:HB3	2.47	0.49
1:D:618:GLY:HA2	1:D:619:ASN:HA	1.61	0.49
1:B:872:ARG:O	1:B:875:VAL:HG12	2.12	0.49
1:B:918:TYR:CD1	1:B:921:SER:HB3	2.47	0.49
1:C:468:ASP:N	1:C:469:ILE:HA	2.23	0.48
1:D:516:THR:HG22	1:D:517:ALA:N	2.28	0.48
1:A:863:LEU:HA	1:A:866:ILE:HG22	1.95	0.48
1:A:1047:GLN:HA	1:A:1050:ARG:NH2	2.28	0.48
1:B:446:LYS:HA	1:B:447:LYS:HA	1.54	0.48
1:A:730:LEU:HA	1:A:842:TYR:CE2	2.48	0.48
1:D:872:ARG:O	1:D:875:VAL:HG12	2.12	0.48
1:D:863:LEU:HA	1:D:866:ILE:HG22	1.96	0.48
1:B:818:PHE:HD1	1:B:819:VAL:HG22	1.78	0.48
1:A:872:ARG:O	1:A:875:VAL:HG12	2.12	0.48
1:A:918:TYR:CD1	1:A:921:SER:HB3	2.48	0.48
1:D:730:LEU:HA	1:D:842:TYR:CE2	2.49	0.48
1:C:863:LEU:HA	1:C:866:ILE:HG22	1.95	0.48
1:D:745:ALA:O	1:D:746:PHE:HB2	2.14	0.48
1:D:1047:GLN:HA	1:D:1050:ARG:NH2	2.28	0.48
1:B:981:GLU:O	1:B:984:THR:HG22	2.12	0.48
1:A:629:TYR:HA	1:A:697:LEU:HD21	1.96	0.48
1:A:818:PHE:HD1	1:A:819:VAL:HG22	1.78	0.48
1:A:745:ALA:O	1:A:746:PHE:HB2	2.14	0.48
1:B:863:LEU:HA	1:B:866:ILE:HG22	1.95	0.48
1:C:629:TYR:HA	1:C:697:LEU:HD21	1.96	0.48
1:C:818:PHE:HD1	1:C:819:VAL:HG22	1.78	0.48
1:A:591:LYS:N	1:A:591:LYS:HD2	2.29	0.48
1:B:730:LEU:HA	1:B:842:TYR:CE2	2.49	0.47
1:D:818:PHE:HD1	1:D:819:VAL:HG22	1.78	0.47
1:B:591:LYS:HD2	1:B:591:LYS:N	2.29	0.47
1:C:981:GLU:O	1:C:984:THR:HG22	2.13	0.47
1:B:1048:LYS:HZ1	1:C:1050:ARG:NH1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:629:TYR:HA	1:D:697:LEU:HD21	1.96	0.47
1:C:730:LEU:HA	1:C:842:TYR:CE2	2.49	0.47
1:D:867:LEU:O	1:D:870:LEU:HB3	2.15	0.47
1:A:819:VAL:HG12	1:A:819:VAL:O	2.14	0.47
1:C:591:LYS:HD2	1:C:591:LYS:N	2.29	0.47
1:B:856:CYS:O	1:B:859:PHE:N	2.46	0.47
1:C:867:LEU:O	1:C:870:LEU:HB3	2.15	0.47
1:D:1061:GLN:HE22	1:C:1061:GLN:NE2	2.11	0.47
1:B:629:TYR:HA	1:B:697:LEU:HD21	1.96	0.47
1:A:1066:LYS:HA	1:A:1069:ILE:HD12	1.97	0.47
1:A:649:LYS:HA	1:A:1005:VAL:O	2.15	0.47
1:C:745:ALA:O	1:C:746:PHE:HB2	2.14	0.47
1:D:820:LEU:HD23	1:D:820:LEU:HA	1.74	0.47
1:C:516:THR:HG22	1:C:517:ALA:N	2.28	0.47
1:C:1042:MET:C	1:C:1042:MET:SD	2.93	0.47
1:B:922:PHE:HD1	1:B:922:PHE:N	2.13	0.47
1:C:547:ASP:N	1:C:547:ASP:OD1	2.48	0.47
1:C:690:VAL:HG21	1:C:977:ALA:HB2	1.97	0.47
1:A:547:ASP:N	1:A:547:ASP:OD1	2.48	0.47
1:B:1042:MET:SD	1:B:1042:MET:C	2.93	0.47
1:D:1048:LYS:HZ1	1:A:1050:ARG:HH12	1.63	0.47
1:D:1051:LEU:CD1	1:A:1047:GLN:HE21	2.11	0.47
1:A:1051:LEU:CD1	1:B:1047:GLN:HE21	2.11	0.47
1:B:819:VAL:HG12	1:B:819:VAL:O	2.14	0.47
1:C:693:ASN:O	1:C:695:ILE:HG22	2.14	0.47
1:A:516:THR:HG22	1:A:517:ALA:N	2.27	0.47
1:C:640:PHE:CD2	1:C:642:MET:HB3	2.47	0.47
1:B:878:ILE:HD12	1:B:878:ILE:HA	1.80	0.47
1:A:690:VAL:HG21	1:A:977:ALA:HB2	1.97	0.47
1:A:867:LEU:O	1:A:870:LEU:HB3	2.15	0.47
1:B:867:LEU:O	1:B:870:LEU:HB3	2.15	0.47
1:A:812:TYR:O	1:A:816:ILE:HG12	2.15	0.47
1:B:812:TYR:O	1:B:816:ILE:HG12	2.15	0.47
1:A:922:PHE:N	1:A:922:PHE:CD1	2.83	0.47
1:A:446:LYS:HA	1:A:447:LYS:HA	1.54	0.47
1:C:922:PHE:N	1:C:922:PHE:HD1	2.13	0.47
1:C:819:VAL:HG12	1:C:819:VAL:O	2.14	0.47
1:D:819:VAL:O	1:D:819:VAL:HG12	2.14	0.47
1:D:923:LEU:HD11	1:A:897:PRO:HB3	1.97	0.47
1:B:690:VAL:HG21	1:B:977:ALA:HB2	1.97	0.47
1:B:649:LYS:HA	1:B:1005:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:652:ARG:NH1	1:D:702:VAL:O	2.42	0.47
1:A:839:VAL:O	1:A:842:TYR:HB3	2.15	0.47
1:D:615:ASN:HA	1:D:616:SER:HA	1.50	0.47
1:B:693:ASN:O	1:B:695:ILE:HG22	2.14	0.47
1:A:693:ASN:O	1:A:695:ILE:HG22	2.14	0.47
1:D:591:LYS:HD2	1:D:591:LYS:N	2.29	0.47
1:D:690:VAL:HG21	1:D:977:ALA:HB2	1.97	0.47
1:A:808:GLU:O	1:A:812:TYR:HD2	1.97	0.47
1:A:922:PHE:N	1:A:922:PHE:HD1	2.13	0.47
1:D:534:LEU:HD22	1:D:570:HIS:ND1	2.30	0.47
1:D:589:HIS:O	1:D:591:LYS:NZ	2.39	0.47
1:B:742:PRO:HA	1:B:832:TRP:HE1	1.80	0.47
1:B:1066:LYS:HA	1:B:1069:ILE:HD12	1.97	0.47
1:B:659:ASN:C	1:B:660:PHE:HD1	2.19	0.47
1:C:1042:MET:O	1:C:1045:LEU:N	2.48	0.47
1:B:1042:MET:O	1:B:1045:LEU:N	2.48	0.47
1:B:808:GLU:O	1:B:812:TYR:HD2	1.97	0.47
1:C:922:PHE:N	1:C:922:PHE:CD1	2.83	0.47
1:A:1042:MET:SD	1:A:1042:MET:C	2.93	0.47
1:D:693:ASN:O	1:D:695:ILE:HG22	2.14	0.46
1:D:742:PRO:HA	1:D:832:TRP:HE1	1.81	0.46
1:C:1066:LYS:HA	1:C:1069:ILE:HD12	1.97	0.46
1:D:526:TYR:O	1:D:530:MET:HE3	2.15	0.46
1:B:652:ARG:NH1	1:B:702:VAL:O	2.41	0.46
1:A:682:PRO:O	1:A:683:LEU:HB2	2.15	0.46
1:D:922:PHE:HD1	1:D:922:PHE:N	2.13	0.46
1:D:1057:LEU:O	1:D:1057:LEU:HD23	2.15	0.46
1:C:534:LEU:HD22	1:C:570:HIS:ND1	2.30	0.46
1:B:658:TYR:N	1:B:659:ASN:HA	2.30	0.46
1:B:707:LEU:O	1:B:711:TRP:HB2	2.16	0.46
1:B:534:LEU:HD22	1:B:570:HIS:ND1	2.30	0.46
1:D:1042:MET:O	1:D:1045:LEU:N	2.48	0.46
1:A:534:LEU:HD22	1:A:570:HIS:ND1	2.30	0.46
1:B:745:ALA:O	1:B:746:PHE:HB2	2.14	0.46
1:C:649:LYS:HA	1:C:1005:VAL:O	2.15	0.46
1:D:649:LYS:HA	1:D:1005:VAL:O	2.15	0.46
1:D:1074:ILE:H	1:A:458:ARG:NH2	2.13	0.46
1:C:659:ASN:C	1:C:660:PHE:HD1	2.19	0.46
1:D:658:TYR:N	1:D:659:ASN:HA	2.30	0.46
1:B:547:ASP:OD1	1:B:547:ASP:N	2.48	0.46
1:B:839:VAL:O	1:B:842:TYR:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:839:VAL:O	1:D:842:TYR:HB3	2.15	0.46
1:D:468:ASP:N	1:D:469:ILE:HA	2.23	0.46
1:A:658:TYR:N	1:A:659:ASN:HA	2.30	0.46
1:A:1042:MET:O	1:A:1045:LEU:N	2.48	0.46
1:D:1042:MET:C	1:D:1042:MET:SD	2.93	0.46
1:A:557:ARG:O	1:A:592:ARG:NE	2.48	0.46
1:A:1057:LEU:HD23	1:A:1057:LEU:O	2.15	0.46
1:C:557:ARG:O	1:C:592:ARG:NE	2.48	0.46
1:C:839:VAL:O	1:C:842:TYR:HB3	2.15	0.46
1:A:742:PRO:HA	1:A:832:TRP:HE1	1.80	0.46
1:A:496:LYS:HA	1:A:496:LYS:HZ3	1.80	0.46
1:D:659:ASN:C	1:D:660:PHE:HD1	2.19	0.46
1:B:602:SER:HA	1:B:603:LYS:HA	1.48	0.46
1:C:808:GLU:O	1:C:812:TYR:HD2	1.97	0.46
1:C:742:PRO:HA	1:C:832:TRP:HE1	1.80	0.46
1:A:550:THR:O	1:A:553:HIS:N	2.48	0.46
1:B:550:THR:O	1:B:553:HIS:N	2.48	0.46
1:D:922:PHE:N	1:D:922:PHE:CD1	2.83	0.46
1:C:682:PRO:O	1:C:683:LEU:HB2	2.15	0.46
1:D:808:GLU:O	1:D:812:TYR:HD2	1.97	0.46
1:D:812:TYR:O	1:D:816:ILE:HG12	2.15	0.46
1:A:659:ASN:C	1:A:660:PHE:HD1	2.19	0.46
1:D:707:LEU:O	1:D:711:TRP:HB2	2.16	0.46
1:B:682:PRO:O	1:B:683:LEU:HB2	2.15	0.46
1:D:632:GLU:OE1	1:D:700:HIS:ND1	2.49	0.46
1:A:1074:ILE:H	1:B:458:ARG:NH2	2.14	0.46
1:C:707:LEU:O	1:C:711:TRP:HB2	2.16	0.46
1:D:820:LEU:O	1:D:823:PHE:N	2.46	0.46
1:D:547:ASP:OD1	1:D:547:ASP:N	2.48	0.46
1:A:632:GLU:OE1	1:A:700:HIS:ND1	2.49	0.46
1:D:1066:LYS:HA	1:D:1069:ILE:HD12	1.97	0.46
1:A:707:LEU:O	1:A:711:TRP:HB2	2.16	0.46
1:B:557:ARG:O	1:B:592:ARG:NE	2.48	0.46
1:A:856:CYS:O	1:A:858:ILE:N	2.49	0.46
1:B:526:TYR:O	1:B:530:MET:HE3	2.16	0.46
1:B:922:PHE:N	1:B:922:PHE:CD1	2.83	0.46
1:C:1057:LEU:O	1:C:1057:LEU:HD23	2.15	0.46
1:B:1051:LEU:HD22	1:C:1047:GLN:HE22	1.82	0.45
1:B:913:LEU:HD12	1:B:913:LEU:O	2.17	0.45
1:A:815:GLY:O	1:A:818:PHE:HB3	2.16	0.45
1:A:640:PHE:CD2	1:A:642:MET:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:640:PHE:CD2	1:D:642:MET:HB3	2.47	0.45
1:C:913:LEU:O	1:C:913:LEU:HD12	2.17	0.45
1:C:856:CYS:O	1:C:858:ILE:N	2.49	0.45
1:B:808:GLU:O	1:B:812:TYR:CD2	2.70	0.45
1:C:812:TYR:O	1:C:816:ILE:HG12	2.15	0.45
1:D:852:ARG:HD3	1:D:982:LEU:HG	1.98	0.45
1:D:682:PRO:O	1:D:683:LEU:HB2	2.15	0.45
1:C:652:ARG:NH1	1:C:702:VAL:O	2.42	0.45
1:D:446:LYS:HA	1:D:447:LYS:HA	1.54	0.45
1:B:632:GLU:OE1	1:B:700:HIS:ND1	2.49	0.45
1:D:815:GLY:O	1:D:818:PHE:HB3	2.16	0.45
1:C:925:PRO:O	1:C:929:ASN:N	2.48	0.45
1:C:658:TYR:N	1:C:659:ASN:HA	2.30	0.45
1:A:526:TYR:O	1:A:530:MET:HE3	2.17	0.45
1:B:533:ILE:O	1:B:536:THR:OG1	2.34	0.45
1:A:913:LEU:HD12	1:A:913:LEU:O	2.17	0.45
1:C:815:GLY:O	1:C:818:PHE:HB3	2.16	0.45
1:C:527:THR:OG1	1:C:528:GLN:N	2.50	0.45
1:D:557:ARG:O	1:D:592:ARG:NE	2.48	0.45
1:A:602:SER:HA	1:A:603:LYS:HA	1.48	0.45
1:A:1048:LYS:HZ1	1:B:1050:ARG:NH1	2.14	0.45
1:D:1050:ARG:HH12	1:C:1048:LYS:HZ1	1.64	0.45
1:C:856:CYS:O	1:C:859:PHE:N	2.46	0.45
1:A:808:GLU:O	1:A:812:TYR:CD2	2.70	0.45
1:B:815:GLY:O	1:B:818:PHE:HB3	2.16	0.45
1:D:856:CYS:O	1:D:858:ILE:N	2.49	0.45
1:B:852:ARG:O	1:B:853:PHE:HB2	2.16	0.45
1:A:615:ASN:HA	1:A:616:SER:HA	1.50	0.45
1:C:820:LEU:O	1:C:823:PHE:N	2.46	0.45
1:C:533:ILE:O	1:C:536:THR:OG1	2.34	0.45
1:D:533:ILE:O	1:D:536:THR:OG1	2.34	0.45
1:A:876:VAL:HG11	1:B:859:PHE:CE2	2.52	0.45
1:C:808:GLU:O	1:C:812:TYR:CD2	2.70	0.45
1:A:852:ARG:O	1:A:853:PHE:HB2	2.16	0.45
1:C:852:ARG:O	1:C:853:PHE:HB2	2.16	0.45
1:B:1057:LEU:O	1:B:1057:LEU:HD23	2.15	0.45
1:A:1051:LEU:HD22	1:B:1047:GLN:HE22	1.82	0.45
1:B:516:THR:HG22	1:B:517:ALA:N	2.27	0.45
1:A:871:LEU:HA	1:A:874:THR:HG22	1.99	0.45
1:A:553:HIS:ND1	1:A:583:PHE:HB3	2.32	0.45
1:A:618:GLY:HA2	1:A:619:ASN:HA	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:THR:OG1	1:D:528:GLN:N	2.50	0.45
1:B:631:PRO:O	1:B:632:GLU:C	2.56	0.44
1:C:631:PRO:O	1:C:632:GLU:C	2.56	0.44
1:C:632:GLU:OE1	1:C:700:HIS:ND1	2.49	0.44
1:C:878:ILE:HA	1:C:878:ILE:HD12	1.80	0.44
1:C:526:TYR:O	1:C:530:MET:HE3	2.16	0.44
1:B:852:ARG:HD3	1:B:982:LEU:HG	1.98	0.44
1:A:533:ILE:O	1:A:536:THR:OG1	2.34	0.44
1:D:553:HIS:ND1	1:D:583:PHE:HB3	2.32	0.44
1:B:856:CYS:O	1:B:858:ILE:N	2.49	0.44
1:D:596:VAL:HA	1:D:599:ILE:HG22	1.99	0.44
1:C:728:LEU:O	1:C:732:PRO:HG2	2.17	0.44
1:C:695:ILE:HB	1:C:973:LEU:HD21	1.99	0.44
1:B:640:PHE:CD2	1:B:642:MET:HB3	2.47	0.44
1:D:852:ARG:O	1:D:853:PHE:HB2	2.16	0.44
1:C:820:LEU:HD23	1:C:820:LEU:HA	1.74	0.44
1:A:695:ILE:HB	1:A:973:LEU:HD21	1.99	0.44
1:D:808:GLU:O	1:D:812:TYR:CD2	2.70	0.44
1:B:695:ILE:HB	1:B:973:LEU:HD21	1.99	0.44
1:D:913:LEU:O	1:D:913:LEU:HD12	2.17	0.44
1:C:852:ARG:HD3	1:C:982:LEU:HG	1.98	0.44
1:C:871:LEU:HA	1:C:874:THR:HG22	1.99	0.44
1:C:553:HIS:ND1	1:C:583:PHE:HB3	2.32	0.44
1:D:550:THR:O	1:D:553:HIS:N	2.48	0.44
1:A:652:ARG:NH1	1:A:702:VAL:O	2.42	0.44
1:A:596:VAL:HA	1:A:599:ILE:HG22	1.99	0.44
1:B:728:LEU:O	1:B:732:PRO:HG2	2.17	0.44
1:A:558:GLU:H	1:A:558:GLU:HG2	1.64	0.44
1:D:1048:LYS:HZ3	1:A:1050:ARG:HH22	1.64	0.44
1:D:631:PRO:O	1:D:632:GLU:C	2.56	0.44
1:D:458:ARG:NH2	1:C:1074:ILE:H	2.15	0.44
1:D:886:LEU:O	1:D:889:TYR:HB3	2.18	0.44
1:C:496:LYS:HA	1:C:496:LYS:HZ2	1.81	0.44
1:B:553:HIS:ND1	1:B:583:PHE:HB3	2.32	0.44
1:B:876:VAL:HG11	1:C:859:PHE:CE2	2.53	0.44
1:A:527:THR:OG1	1:A:528:GLN:N	2.50	0.44
1:C:446:LYS:HA	1:C:447:LYS:HA	1.54	0.44
1:A:631:PRO:O	1:A:632:GLU:C	2.56	0.44
1:B:615:ASN:HA	1:B:616:SER:HA	1.50	0.44
1:B:886:LEU:O	1:B:889:TYR:HB3	2.18	0.44
1:C:886:LEU:O	1:C:889:TYR:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:518:LEU:HD11	1:D:530:MET:HG3	2.00	0.44
1:B:527:THR:OG1	1:B:528:GLN:N	2.50	0.44
1:B:871:LEU:HA	1:B:874:THR:HG22	1.99	0.44
1:D:695:ILE:HB	1:D:973:LEU:HD21	1.99	0.43
1:B:1042:MET:O	1:B:1043:GLU:C	2.57	0.43
1:A:852:ARG:HD3	1:A:982:LEU:HG	1.98	0.43
1:C:596:VAL:HA	1:C:599:ILE:HG22	1.99	0.43
1:C:518:LEU:HD11	1:C:530:MET:HG3	2.00	0.43
1:A:710:LYS:HG3	1:A:711:TRP:H	1.83	0.43
1:D:768:TYR:O	1:D:772:THR:HG23	2.18	0.43
1:A:728:LEU:O	1:A:732:PRO:HG2	2.17	0.43
1:D:728:LEU:O	1:D:732:PRO:HG2	2.17	0.43
1:D:933:HIS:NE2	1:A:833:GLN:CB	2.81	0.43
1:D:1047:GLN:HE22	1:C:1051:LEU:HD22	1.83	0.43
1:D:871:LEU:HA	1:D:874:THR:HG22	1.99	0.43
1:D:856:CYS:O	1:D:859:PHE:N	2.46	0.43
1:A:709:MET:O	1:A:712:LEU:HB3	2.18	0.43
1:A:768:TYR:O	1:A:772:THR:HG23	2.19	0.43
1:D:709:MET:O	1:D:712:LEU:HB3	2.18	0.43
1:B:496:LYS:HZ2	1:B:496:LYS:HA	1.80	0.43
1:B:621:CYS:SG	1:B:622:PRO:HD3	2.58	0.43
1:A:621:CYS:SG	1:A:622:PRO:HD3	2.58	0.43
1:B:710:LYS:HG3	1:B:711:TRP:H	1.84	0.43
1:A:1042:MET:O	1:A:1043:GLU:C	2.57	0.43
1:A:818:PHE:HD2	1:A:835:GLY:CA	2.32	0.43
1:C:743:GLY:N	1:C:832:TRP:HE1	2.14	0.43
1:C:768:TYR:O	1:C:772:THR:HG23	2.18	0.43
1:C:502:LEU:HA	1:C:505:GLY:HA2	2.01	0.43
1:C:1070:GLN:NE2	1:C:1070:GLN:O	2.52	0.43
1:A:997:LYS:CB	1:A:998:VAL:HA	2.46	0.43
1:B:618:GLY:HA2	1:B:619:ASN:HA	1.61	0.43
1:C:709:MET:O	1:C:712:LEU:HB3	2.19	0.43
1:C:656:ILE:HG13	1:C:656:ILE:H	1.64	0.43
1:B:1074:ILE:H	1:C:458:ARG:NH2	2.17	0.43
1:D:874:THR:O	1:D:878:ILE:HB	2.19	0.43
1:C:710:LYS:HG3	1:C:711:TRP:H	1.84	0.43
1:B:596:VAL:HA	1:B:599:ILE:HG22	1.99	0.43
1:D:632:GLU:OE1	1:D:632:GLU:HA	2.19	0.43
1:B:818:PHE:HD2	1:B:835:GLY:CA	2.32	0.43
1:B:997:LYS:CB	1:B:998:VAL:HA	2.46	0.43
1:C:457:GLY:HA3	1:C:494:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:621:CYS:SG	1:D:622:PRO:HD3	2.58	0.43
1:B:611:ILE:O	1:B:612:PHE:HB2	2.19	0.43
1:B:709:MET:O	1:B:712:LEU:HB3	2.18	0.43
1:D:502:LEU:HA	1:D:505:GLY:HA2	2.01	0.43
1:C:611:ILE:O	1:C:612:PHE:HB2	2.19	0.43
1:A:632:GLU:OE1	1:A:632:GLU:HA	2.19	0.43
1:A:874:THR:O	1:A:878:ILE:HB	2.19	0.43
1:C:1042:MET:O	1:C:1043:GLU:C	2.57	0.43
1:D:1070:GLN:O	1:D:1070:GLN:NE2	2.52	0.43
1:B:632:GLU:OE1	1:B:632:GLU:HA	2.19	0.43
1:B:925:PRO:O	1:B:929:ASN:N	2.48	0.43
1:B:730:LEU:N	1:B:842:TYR:OH	2.52	0.43
1:A:730:LEU:N	1:A:842:TYR:OH	2.52	0.43
1:C:931:LEU:HD12	1:C:931:LEU:O	2.19	0.43
1:D:457:GLY:HA3	1:D:494:HIS:CD2	2.54	0.43
1:B:518:LEU:HD11	1:B:530:MET:HG3	2.00	0.43
1:C:621:CYS:SG	1:C:622:PRO:HD3	2.58	0.43
1:A:603:LYS:HE2	1:A:603:LYS:HB2	1.77	0.43
1:D:936:LEU:HD13	1:A:837:ILE:HD11	2.01	0.43
1:B:502:LEU:HA	1:B:505:GLY:HA2	2.01	0.43
1:D:730:LEU:N	1:D:842:TYR:OH	2.52	0.42
1:C:895:GLN:NE2	1:C:896:ASP:O	2.52	0.42
1:A:502:LEU:HA	1:A:505:GLY:HA2	2.01	0.42
1:D:909:PHE:CE2	1:C:942:VAL:HG23	2.54	0.42
1:D:1051:LEU:HD22	1:A:1047:GLN:HE22	1.84	0.42
1:A:811:ILE:HD12	1:A:842:TYR:HA	2.01	0.42
1:B:695:ILE:HG21	1:B:973:LEU:HD11	2.02	0.42
1:C:695:ILE:HG21	1:C:973:LEU:HD11	2.02	0.42
1:A:886:LEU:O	1:A:889:TYR:HB3	2.18	0.42
1:D:916:ILE:CG2	1:D:919:ARG:HB2	2.50	0.42
1:B:457:GLY:HA3	1:B:494:HIS:CD2	2.54	0.42
1:A:518:LEU:HD11	1:A:530:MET:HG3	2.00	0.42
1:D:611:ILE:O	1:D:612:PHE:HB2	2.19	0.42
1:A:1070:GLN:O	1:A:1070:GLN:NE2	2.52	0.42
1:D:629:TYR:N	1:D:697:LEU:HD11	2.23	0.42
1:D:695:ILE:HG21	1:D:973:LEU:HD11	2.02	0.42
1:B:973:LEU:HA	1:B:973:LEU:HD23	1.86	0.42
1:D:743:GLY:N	1:D:832:TRP:HE1	2.14	0.42
1:C:874:THR:O	1:C:878:ILE:HB	2.19	0.42
1:D:584:LEU:HD22	1:D:619:ASN:OD1	2.20	0.42
1:C:584:LEU:HD22	1:C:619:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1048:LYS:HZ1	1:A:1050:ARG:NH1	2.17	0.42
1:B:811:ILE:HD12	1:B:842:TYR:HA	2.01	0.42
1:C:730:LEU:N	1:C:842:TYR:OH	2.52	0.42
1:B:468:ASP:N	1:B:469:ILE:HA	2.23	0.42
1:C:719:HIS:NE2	1:C:852:ARG:HD2	2.35	0.42
1:D:895:GLN:NE2	1:D:896:ASP:O	2.52	0.42
1:D:850:LEU:HD23	1:D:850:LEU:HA	1.79	0.42
1:B:829:HIS:ND1	1:B:829:HIS:C	2.73	0.42
1:A:990:LEU:HA	1:A:991:PRO:HD3	1.88	0.42
1:D:597:LEU:HD13	1:D:601:ARG:HH12	1.84	0.42
1:D:736:LEU:HD13	1:D:773:CYS:SG	2.60	0.42
1:A:611:ILE:O	1:A:612:PHE:HB2	2.19	0.42
1:B:768:TYR:O	1:B:772:THR:HG23	2.18	0.42
1:D:818:PHE:HD2	1:D:835:GLY:CA	2.32	0.42
1:A:695:ILE:HG21	1:A:973:LEU:HD11	2.02	0.42
1:B:874:THR:O	1:B:878:ILE:HB	2.19	0.42
1:A:916:ILE:CG2	1:A:919:ARG:HB2	2.50	0.42
1:C:948:VAL:HB	1:C:949:PRO:HD3	2.02	0.42
1:B:719:HIS:NE2	1:B:852:ARG:HD2	2.35	0.42
1:D:931:LEU:O	1:D:931:LEU:HD12	2.19	0.42
1:B:948:VAL:HB	1:B:949:PRO:HD3	2.02	0.42
1:A:584:LEU:HD22	1:A:619:ASN:OD1	2.20	0.42
1:A:719:HIS:NE2	1:A:852:ARG:HD2	2.35	0.42
1:B:1070:GLN:O	1:B:1070:GLN:NE2	2.52	0.42
1:C:512:HIS:C	1:C:512:HIS:CD2	2.93	0.42
1:C:632:GLU:HA	1:C:632:GLU:OE1	2.19	0.42
1:B:931:LEU:O	1:B:931:LEU:HD12	2.20	0.42
1:D:948:VAL:HB	1:D:949:PRO:HD3	2.02	0.42
1:A:457:GLY:HA3	1:A:494:HIS:CD2	2.54	0.42
1:A:597:LEU:HD13	1:A:601:ARG:HH12	1.84	0.42
1:D:1042:MET:O	1:D:1043:GLU:C	2.57	0.42
1:A:829:HIS:C	1:A:829:HIS:ND1	2.72	0.42
1:A:931:LEU:O	1:A:931:LEU:HD12	2.19	0.42
1:C:916:ILE:CG2	1:C:919:ARG:HB2	2.49	0.42
1:B:916:ILE:CG2	1:B:919:ARG:HB2	2.49	0.42
1:D:710:LYS:HG3	1:D:711:TRP:H	1.84	0.42
1:C:736:LEU:HD13	1:C:773:CYS:SG	2.60	0.42
1:D:602:SER:HA	1:D:603:LYS:HA	1.48	0.42
1:D:829:HIS:C	1:D:829:HIS:ND1	2.73	0.42
1:A:923:LEU:CD1	1:B:897:PRO:HB3	2.50	0.42
1:D:874:THR:HA	1:D:877:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:THR:O	1:C:553:HIS:N	2.47	0.42
1:A:895:GLN:NE2	1:A:896:ASP:O	2.52	0.42
1:C:829:HIS:C	1:C:829:HIS:ND1	2.73	0.42
1:D:512:HIS:C	1:D:512:HIS:CD2	2.93	0.42
1:C:629:TYR:N	1:C:697:LEU:HD11	2.23	0.41
1:A:970:HIS:HE1	1:A:974:LYS:NZ	2.18	0.41
1:B:975:ARG:HG2	1:B:976:ILE:HD13	2.02	0.41
1:C:580:GLN:HG3	1:C:615:ASN:O	2.20	0.41
1:A:949:PRO:HB3	1:B:913:LEU:CD1	2.50	0.41
1:D:684:THR:O	1:D:687:ASN:HB3	2.20	0.41
1:B:862:MET:SD	1:B:964:ILE:HG23	2.60	0.41
1:C:684:THR:O	1:C:687:ASN:HB3	2.20	0.41
1:A:719:HIS:CD2	1:A:852:ARG:HD2	2.55	0.41
1:A:731:ILE:HG13	1:A:731:ILE:H	1.69	0.41
1:A:874:THR:HA	1:A:877:PHE:CE2	2.55	0.41
1:A:948:VAL:HB	1:A:949:PRO:HD3	2.02	0.41
1:B:949:PRO:HB3	1:C:913:LEU:CD1	2.50	0.41
1:B:736:LEU:HD13	1:B:773:CYS:SG	2.60	0.41
1:A:736:LEU:HD13	1:A:773:CYS:SG	2.60	0.41
1:A:512:HIS:C	1:A:512:HIS:CD2	2.93	0.41
1:A:919:ARG:O	1:A:919:ARG:HG3	2.20	0.41
1:A:891:LEU:O	1:A:892:LEU:HD13	2.20	0.41
1:C:597:LEU:HD13	1:C:601:ARG:HH12	1.84	0.41
1:D:719:HIS:CD2	1:D:852:ARG:HD2	2.55	0.41
1:A:923:LEU:CD2	1:B:897:PRO:HG3	2.49	0.41
1:B:919:ARG:HG3	1:B:919:ARG:O	2.20	0.41
1:C:891:LEU:O	1:C:892:LEU:HD13	2.20	0.41
1:D:862:MET:SD	1:D:964:ILE:HG23	2.60	0.41
1:B:895:GLN:NE2	1:B:896:ASP:O	2.52	0.41
1:A:635:LYS:HB2	1:A:635:LYS:HE2	1.81	0.41
1:B:580:GLN:HG3	1:B:615:ASN:O	2.20	0.41
1:C:975:ARG:HG2	1:C:976:ILE:HD13	2.02	0.41
1:A:580:GLN:HG3	1:A:615:ASN:O	2.20	0.41
1:B:638:LEU:HD21	1:B:653:ASP:O	2.21	0.41
1:B:595:VAL:O	1:B:598:THR:HG22	2.21	0.41
1:C:919:ARG:HG3	1:C:919:ARG:O	2.20	0.41
1:D:997:LYS:CB	1:D:998:VAL:HA	2.46	0.41
1:B:584:LEU:HD22	1:B:619:ASN:OD1	2.20	0.41
1:B:554:PHE:O	1:B:557:ARG:N	2.54	0.41
1:D:1050:ARG:NH1	1:C:1048:LYS:HZ1	2.18	0.41
1:B:970:HIS:HE1	1:B:974:LYS:NZ	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:835:GLY:O	1:D:839:VAL:HG23	2.21	0.41
1:C:874:THR:HA	1:C:877:PHE:CE2	2.55	0.41
1:A:862:MET:SD	1:A:964:ILE:HG23	2.60	0.41
1:B:1075:ILE:HA	1:B:1076:SER:HA	1.94	0.41
1:D:635:LYS:HE2	1:D:635:LYS:HB2	1.81	0.41
1:B:512:HIS:C	1:B:512:HIS:CD2	2.93	0.41
1:A:835:GLY:O	1:A:839:VAL:HG23	2.21	0.41
1:D:859:PHE:CE2	1:C:876:VAL:HG11	2.55	0.41
1:D:719:HIS:NE2	1:D:852:ARG:HD2	2.35	0.41
1:B:835:GLY:O	1:B:839:VAL:HG23	2.21	0.41
1:A:468:ASP:N	1:A:469:ILE:HA	2.23	0.41
1:B:874:THR:HA	1:B:877:PHE:CE2	2.55	0.41
1:B:719:HIS:CD2	1:B:852:ARG:HD2	2.55	0.41
1:C:719:HIS:CD2	1:C:852:ARG:HD2	2.55	0.41
1:C:970:HIS:HE1	1:C:974:LYS:NZ	2.18	0.41
1:C:811:ILE:HD12	1:C:842:TYR:HA	2.02	0.41
1:C:835:GLY:O	1:C:839:VAL:HG23	2.21	0.41
1:D:811:ILE:HD12	1:D:842:TYR:HA	2.02	0.41
1:C:638:LEU:HD21	1:C:653:ASP:O	2.21	0.41
1:A:638:LEU:HD21	1:A:653:ASP:O	2.21	0.41
1:D:919:ARG:HG3	1:D:919:ARG:O	2.20	0.41
1:A:684:THR:O	1:A:687:ASN:HB3	2.20	0.41
1:A:856:CYS:O	1:A:859:PHE:N	2.46	0.41
1:A:554:PHE:O	1:A:557:ARG:N	2.54	0.41
1:C:635:LYS:HE2	1:C:635:LYS:HB2	1.81	0.41
1:C:602:SER:HA	1:C:603:LYS:HA	1.48	0.41
1:D:580:GLN:HG3	1:D:615:ASN:O	2.20	0.41
1:A:975:ARG:HG2	1:A:976:ILE:HD13	2.02	0.41
1:B:891:LEU:O	1:B:892:LEU:HD13	2.20	0.41
1:C:862:MET:SD	1:C:964:ILE:HG23	2.60	0.41
1:B:684:THR:O	1:B:687:ASN:HB3	2.20	0.41
1:C:953:MET:O	1:C:957:ILE:HG13	2.21	0.41
1:C:616:SER:HA	1:C:617:PRO:HD3	1.90	0.41
1:C:818:PHE:HD2	1:C:835:GLY:CA	2.32	0.40
1:D:626:MET:O	1:D:627:ILE:HG13	2.21	0.40
1:D:595:VAL:O	1:D:598:THR:HG22	2.21	0.40
1:C:595:VAL:O	1:C:598:THR:HG22	2.21	0.40
1:D:990:LEU:HD21	1:D:994:PHE:HD2	1.86	0.40
1:D:876:VAL:HG11	1:A:859:PHE:CE2	2.56	0.40
1:C:850:LEU:HA	1:C:850:LEU:HD23	1.79	0.40
1:D:970:HIS:HE1	1:D:974:LYS:NZ	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:990:LEU:HD21	1:A:994:PHE:HD2	1.86	0.40
1:D:891:LEU:O	1:D:892:LEU:HD13	2.20	0.40
1:C:851:GLN:HA	1:C:860:ILE:HD13	2.04	0.40
1:D:913:LEU:CD1	1:C:949:PRO:HB3	2.51	0.40
1:D:554:PHE:O	1:D:557:ARG:N	2.54	0.40
1:A:626:MET:O	1:A:627:ILE:HG13	2.21	0.40
1:A:595:VAL:O	1:A:598:THR:HG22	2.21	0.40
1:B:603:LYS:HE2	1:B:603:LYS:HB2	1.77	0.40
1:D:603:LYS:HE2	1:D:603:LYS:HB2	1.77	0.40
1:D:975:ARG:HG2	1:D:976:ILE:HD13	2.02	0.40
1:B:942:VAL:HG23	1:C:909:PHE:CE2	2.57	0.40
1:D:814:THR:HG21	1:D:838:ALA:HA	2.03	0.40
1:D:1050:ARG:HH22	1:C:1048:LYS:HZ3	1.69	0.40
1:D:638:LEU:HD21	1:D:653:ASP:O	2.21	0.40
1:B:990:LEU:HD21	1:B:994:PHE:HD2	1.86	0.40
1:C:990:LEU:HD21	1:C:994:PHE:HD2	1.86	0.40
1:D:851:GLN:HA	1:D:860:ILE:HD13	2.04	0.40
1:D:953:MET:O	1:D:957:ILE:HG13	2.21	0.40
1:D:1067:LEU:O	1:D:1067:LEU:HD13	2.22	0.40
1:B:953:MET:O	1:B:957:ILE:HG13	2.21	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 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	550/1528 (36%)	485 (88%)	56 (10%)	9 (2%)	12	57
1	B	550/1528 (36%)	485 (88%)	56 (10%)	9 (2%)	12	57
1	C	550/1528 (36%)	485 (88%)	56 (10%)	9 (2%)	12	57
1	D	550/1528 (36%)	485 (88%)	56 (10%)	9 (2%)	12	57
All	All	2200/6112 (36%)	1940 (88%)	224 (10%)	36 (2%)	17	57

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	580	GLN
1	D	639	ASP
1	A	580	GLN
1	A	639	ASP
1	B	580	GLN
1	B	639	ASP
1	C	580	GLN
1	C	639	ASP
1	D	746	PHE
1	D	853	PHE
1	D	1075	ILE
1	A	746	PHE
1	A	853	PHE
1	A	1075	ILE
1	B	746	PHE
1	B	853	PHE
1	B	1075	ILE
1	C	746	PHE
1	C	853	PHE
1	C	1075	ILE
1	D	828	ALA
1	D	948	VAL
1	A	828	ALA
1	A	948	VAL
1	B	828	ALA
1	B	948	VAL
1	C	828	ALA
1	C	948	VAL
1	D	684	THR
1	A	684	THR
1	B	684	THR
1	C	684	THR
1	D	821	PRO
1	A	821	PRO
1	B	821	PRO
1	C	821	PRO

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	415/1325 (31%)	405 (98%)	10 (2%)	57	83
1	B	415/1325 (31%)	405 (98%)	10 (2%)	57	83
1	C	415/1325 (31%)	405 (98%)	10 (2%)	57	83
1	D	415/1325 (31%)	405 (98%)	10 (2%)	57	83
All	All	1660/5300 (31%)	1620 (98%)	40 (2%)	60	83

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	480	LEU
1	D	536	THR
1	D	620	LYS
1	D	690	VAL
1	D	706	TYR
1	D	768	TYR
1	D	785	TYR
1	D	829	HIS
1	D	832	TRP
1	D	1042	MET
1	A	480	LEU
1	A	536	THR
1	A	620	LYS
1	A	690	VAL
1	A	706	TYR
1	A	768	TYR
1	A	785	TYR
1	A	829	HIS
1	A	832	TRP
1	A	1042	MET
1	B	480	LEU
1	B	536	THR
1	B	620	LYS
1	B	690	VAL
1	B	706	TYR
1	B	768	TYR
1	B	785	TYR
1	B	829	HIS
1	B	832	TRP
1	B	1042	MET

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Mol	Chain	Res	Type
1	C	480	LEU
1	C	536	THR
1	C	620	LYS
1	C	690	VAL
1	C	706	TYR
1	C	768	TYR
1	C	785	TYR
1	C	829	HIS
1	C	832	TRP
1	C	1042	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	954	ASN
1	D	1047	GLN
1	D	1061	GLN
1	A	1047	GLN
1	B	1047	GLN
1	B	1061	GLN
1	C	1047	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.