



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:26 AM UTC

PDB ID : 3GTQ / pdb_00003gtq
Title : Backtracked RNA polymerase II complex induced by damage
Authors : Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on : 2009-03-27
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

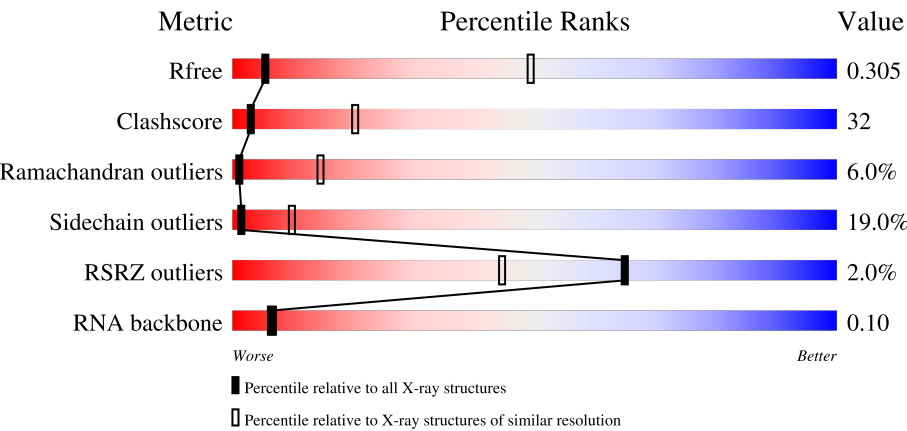
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)
RNA backbone	3983	1007 (4.50-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	1733	2% 35%33%11%•20%
2	B	1224	2% 36%42%12%•10%
3	C	318	33%41%9%•16%
4	E	215	3% 55%35%9%

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Mol	Chain	Length	Quality of chain
5	F	155	
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	
11	R	12	
12	T	29	

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 28625 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 11 is a RNA chain called RNA (5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*GP*A P*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	R	11	Total	C	N	O	P	0	0	0
			243	108	50	74	11			

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*AP*CP*CP*CP*AP*TP*AP*AP *CP*CP*AP*CP*AP*GP*GP*CP*TP*CP*CP*TP*CP*TP*CP*CP*AP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	T	12	Total	C	N	O	P	0	0	0
			234	113	34	75	12			

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total	Zn	0	0
			2	2		

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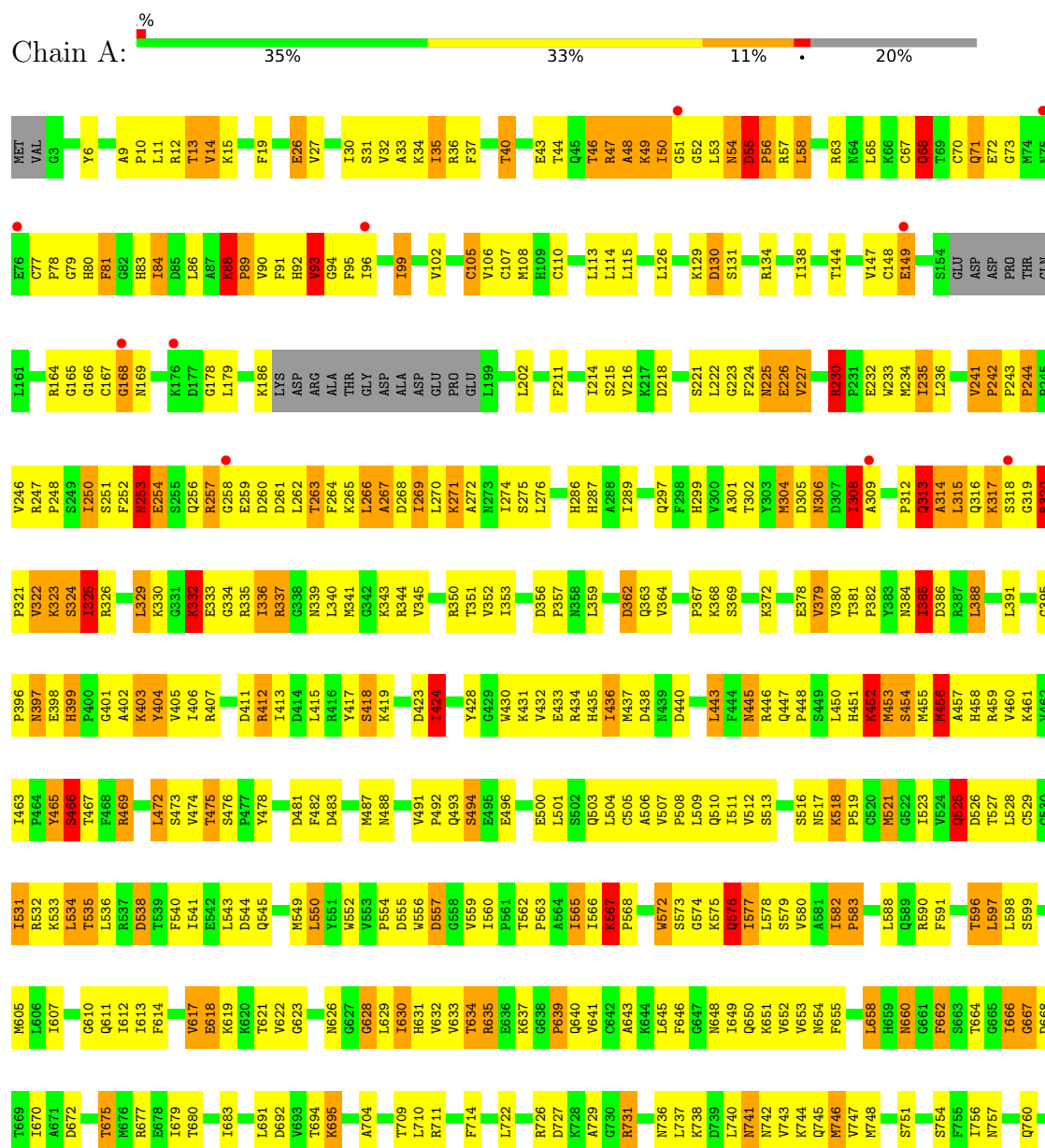
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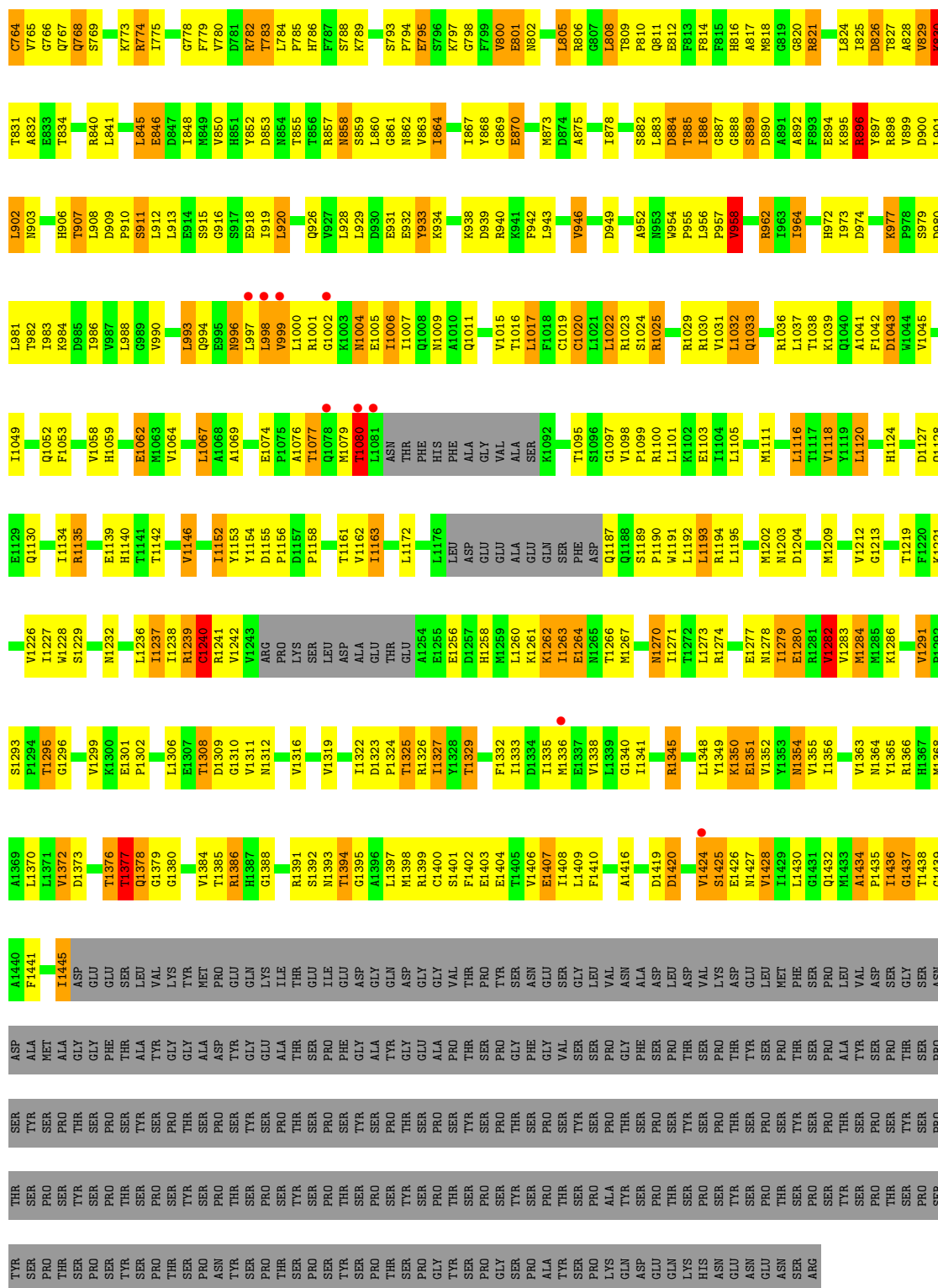
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total 1	Zn 1	0	0
13	C	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	J	1	Total 1	Zn 1	0	0
13	L	1	Total 1	Zn 1	0	0

3 Residue-property plots

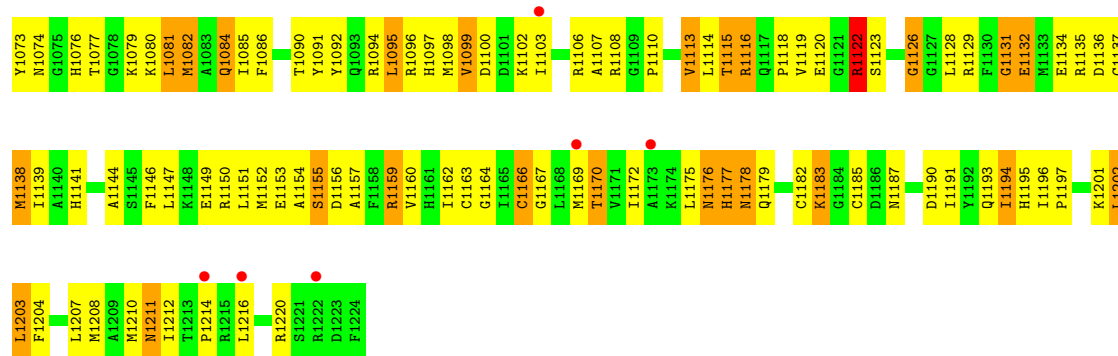
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1



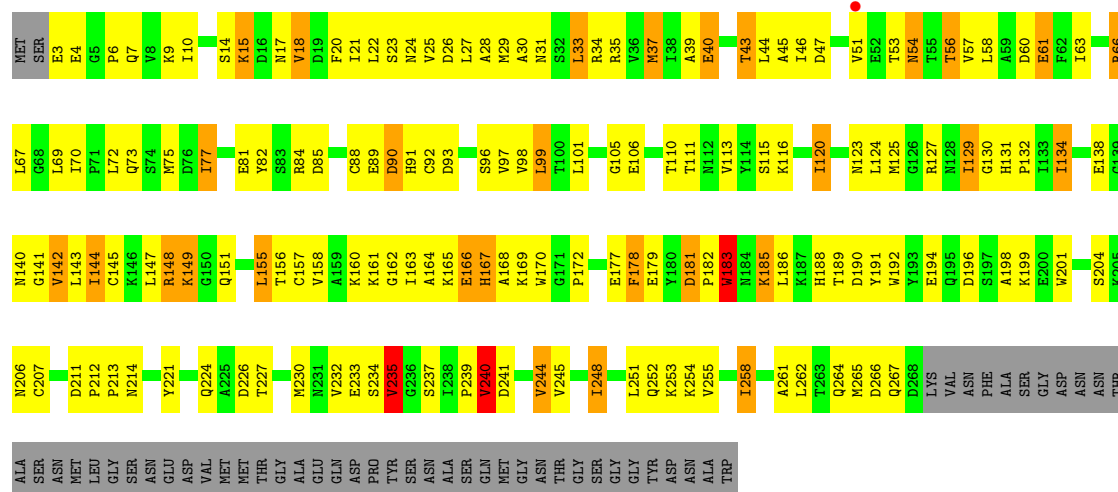


F1001	T1002	A1003	E1004	V1007	P1008	D1009	L1010	I1011	I1012	M1013	P1014	H1015	P1018	S1019	R1020	M1021	T1022	V1023	A1024	H1025	L1026	I1027	E1028	C1029	L1030	L1031	S1032	K1033	I1034	A1035	A1036	L1037	S1045	P1046	F1047	T1048	T1051	G1054	I1055	S1056	L1059	R1060	F1061	H1062	Q1065	S1066	R1067	G1068	F1069	E1070	V1071	M1072																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
THR	ALA	TYR	HIS	R933	R934	R935	D936	A937	S938	T944	E945	T948	V952	L953	V954	T955	T956	N957	Q958	D959	G960	L961	K965	V966	L967	R968	R969	I970	R971	K972	L973	P974	Q975	G977	D978	K979	F980	A981	I982	R983	H984	G985	Q986	G991	I992	T993	Y994	S1066	R1067	R995	G1068	F1069	E1070	V1071	M1072																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
R857	M860	D861	Q862	R863	K864	K865	Y866	S869	I870	T873	T874	F875	E876	R877	Q878	R879	T880	N881	T882	D883	R884	M885	K886	H887	G888	R889	Y890	D894	L898	I899	A900	P901	G902	V903	R904	V910	I911	I912	G913	K914	T915	T916	S919	P920	Q921	G922	Y923	R924	S925	R926	L927	G928	R929	G930	R931	G932	N933	R934	R935	R936	R937	R938	R939	R940	R941	R942	R943	R944	R945	R946	R947	R948	R949	R950	R951	R952	R953	R954	R955	R956	R957	R958	R959	R960	R961	R962	R963	R964	R965	R966	R967	R968	R969	R970	R971	R972	R973	R974	R975	R976	R977	R978	R979	R980	R981	R982	R983	R984	R985	R986	R987	R988	R989	R990	R991	R992	R993	R994	R995	R996	R997	R998	R999	P1000																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
A793	N794	I795	L796	R797	Y798	R799	Q800	R801	L802	P803	L804	G805	T806	R807	H808	C741	H744	P745	S746	M747	L748	L749	G750	V751	S754	I755	I756	D760	H761	N762	Q763	S764	P765	R766	Y769	Q770	S771	A772	M773	A777	M778	G779	V780	F781	L782	T783	N784	Y787	L788	R789	S790	R791	L792	R793	R794	R795	R796	R797	R798	R799	R800	R801	R802	R803	R804	R805	R806	R807	R808	R809	R810	R811	R812	R813	R814	R815	R816	R817	R818	R819	R820	R821	R822	R823	R824	R825	R826	R827	R828	R829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868	R869	R870	R871	R872	R873	R874	R875	R876	R877	R878	R879	R880	R881	R882	R883	R884	R885	R886	R887	R888	R889	R890	R891	R892	R893	R894	R895	R896	R897	R898	R899	R900	R901	R902	R903	R904	R905	R906	R907	R908	R909	R910	R911	R912	R913	R914	R915	R916	R917	R918	R919	R920	R921	R922	R923	R924	R925	R926	R927	R928	R929	R930	R931	R932	R933	R934	R935	R936	R937	R938	R939	R940	R941	R942	R943	R944	R945	R946	R947	R948	R949	R950	R951	R952	R953	R954	R955	R956	R957	R958	R959	R960	R961	R962	R963	R964	R965	R966	R967	R968	R969	R970	R971	R972	R973	R974	R975	R976	R977	R978	R979	R980	R981	R982	R983	R984	R985	R986	R987	R988	R989	R990	R991	R992	R993	R994	R995	R996	R997	R998	R999	P1000																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624	T628	R632	V633	Y634	R635	P636	L637	F638	T639	M640	E641	D642	D643	E644	G647	H648	K649	E650	V653	R654	K655	G656	H657	L658	V585	W586	H587	G588	V589	H590	P593	L596	W597	E598	T599	L600	R601	N610	P611	E612	V613	S614	N615	L616	R617	G618	L619	R620	E621	K622	E623	L624</



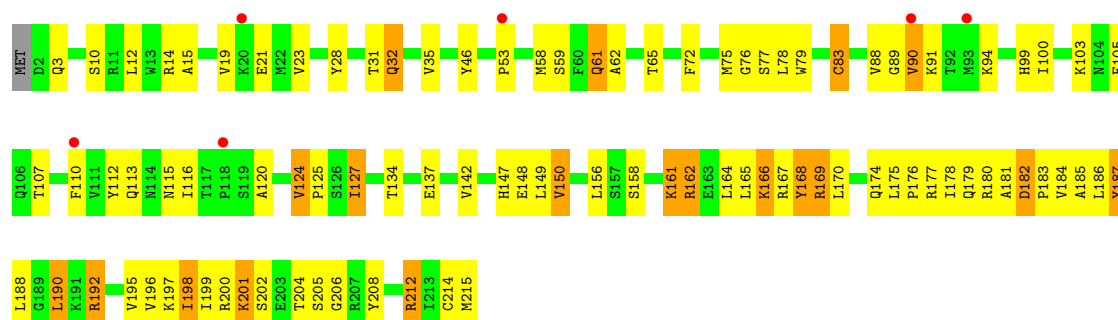
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C: 33% 41% 9% 16%



• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

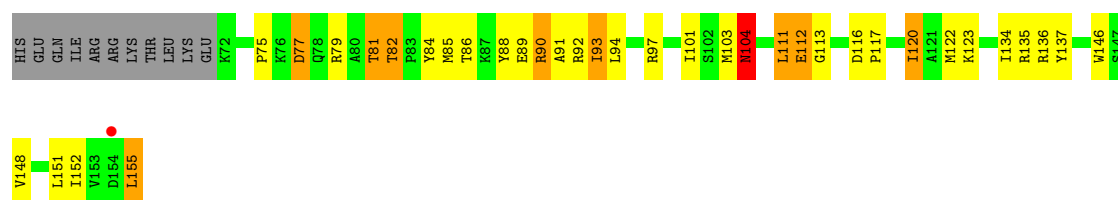
Chain E: 3% 55% 35% 9%



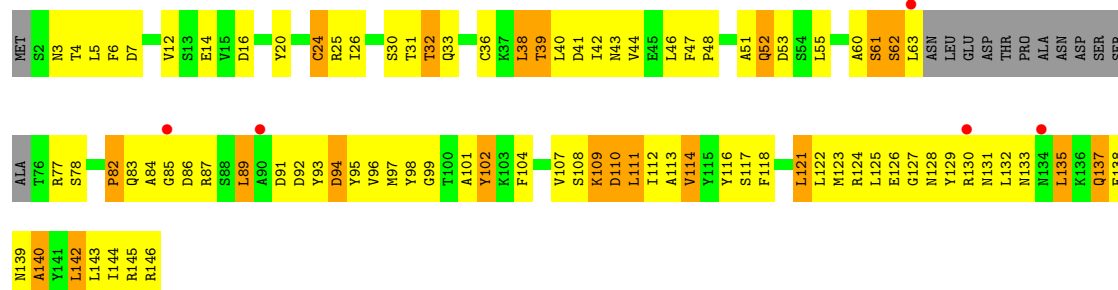
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 31% 17% 6% 46%





- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

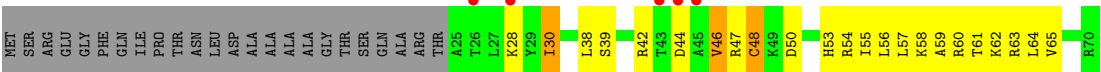
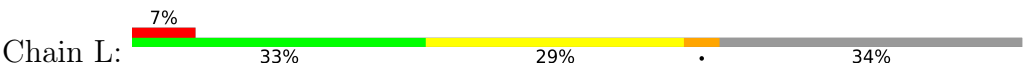


- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

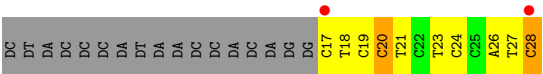
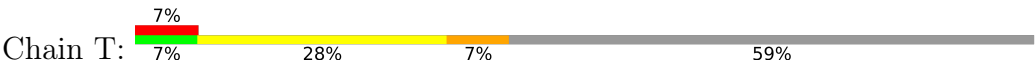




● Molecule 11: RNA (5'-R(P*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*GP*C)-3')



● Molecule 12: DNA (5'-D(*CP*TP*AP*CP*CP*CP*AP*TP*AP*AP*CP*CP*AP*CP*AP*GP*GP*CP*TP*CP*CP*TP*CP*TP*CP*CP*AP*TP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.19Å 221.58Å 192.80Å 90.00° 101.81° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 50.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	95.5 (50.00-3.80) 95.5 (50.00-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.271 , 0.335 0.253 , 0.305	Depositor DCC
R_{free} test set	3287 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	98.0	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	28625	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.70	2/11163 (0.0%)	1.05	36/15091 (0.2%)
2	B	0.73	0/8963	1.06	32/12086 (0.3%)
3	C	0.67	0/2133	1.02	7/2891 (0.2%)
4	E	0.61	0/1788	1.05	8/2406 (0.3%)
5	F	0.66	0/691	0.93	2/933 (0.2%)
6	H	0.64	0/1086	1.02	4/1470 (0.3%)
7	I	0.75	0/989	1.07	7/1331 (0.5%)
8	J	0.71	0/541	1.08	3/727 (0.4%)
9	K	0.64	0/937	0.96	2/1265 (0.2%)
10	L	0.77	0/365	1.08	2/485 (0.4%)
11	R	0.72	0/273	1.30	1/425 (0.2%)
12	T	0.48	0/258	1.56	4/393 (1.0%)
All	All	0.70	2/29187 (0.0%)	1.06	108/39503 (0.3%)

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	2
2	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	474	VAL	CA-CB	6.69	1.63	1.54
1	A	1080	THR	CA-CB	5.10	1.62	1.53

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	161	LYS	N-CA-C	18.79	131.18	111.07
12	T	20	DC	O3'-P-O5'	-9.91	89.14	104.00
2	B	99	LYS	CA-C-N	7.94	129.76	119.84
2	B	99	LYS	C-N-CA	7.94	129.76	119.84
1	A	88	LYS	CA-C-N	7.92	129.74	119.84
1	A	88	LYS	C-N-CA	7.92	129.74	119.84
2	B	777	ALA	N-CA-C	7.83	121.01	108.41
1	A	456	MET	N-CA-C	7.75	120.64	108.79
2	B	647	GLY	N-CA-C	7.73	120.95	112.29
2	B	347	LYS	N-CA-C	-7.67	103.88	113.55
4	E	162	ARG	N-CA-C	-7.67	103.39	112.89
4	E	182	ASP	CA-C-N	7.62	129.37	119.84
4	E	182	ASP	C-N-CA	7.62	129.37	119.84
12	T	20	DC	OP2-P-O3'	-7.49	85.53	108.00
1	A	973	ILE	N-CA-C	7.46	118.56	108.11
1	A	242	PRO	CA-C-N	7.41	125.07	119.66
1	A	242	PRO	C-N-CA	7.41	125.07	119.66
12	T	20	DC	OP1-P-O3'	-7.33	86.03	108.00
2	B	554	ILE	N-CA-C	-7.15	104.76	111.48
2	B	779	GLY	N-CA-C	7.05	120.74	110.80
4	E	162	ARG	N-CA-CB	-7.01	98.97	110.40
3	C	181	ASP	CA-C-N	6.98	128.57	119.84
3	C	181	ASP	C-N-CA	6.98	128.57	119.84
1	A	1311	VAL	N-CA-C	6.97	117.69	107.37
3	C	235	VAL	N-CA-C	-6.76	103.93	110.42
5	F	93	ILE	N-CA-C	-6.74	104.61	110.74
1	A	582	ILE	CA-C-N	6.72	128.24	119.84
1	A	582	ILE	C-N-CA	6.72	128.24	119.84
1	A	1240	CYS	N-CA-C	6.66	119.07	107.49
1	A	230	ARG	CA-C-N	6.58	128.07	119.84
1	A	230	ARG	C-N-CA	6.58	128.07	119.84
2	B	635	ARG	CA-C-N	6.51	127.98	119.84
2	B	635	ARG	C-N-CA	6.51	127.98	119.84
2	B	888	GLY	N-CA-C	6.41	120.48	112.79
1	A	253	ASN	N-CA-C	6.39	124.41	110.80
6	H	137	GLN	N-CA-C	6.32	118.29	109.31
1	A	54	ASN	N-CA-C	6.32	119.89	111.30
2	B	756	ILE	N-CA-C	6.32	114.06	108.63
2	B	778	MET	N-CA-C	6.28	119.09	110.24
1	A	452	LYS	N-CA-C	-6.24	105.95	112.93
8	J	3	VAL	CB-CA-C	-6.23	104.16	110.89
2	B	1122	ARG	N-CA-C	-6.23	104.95	113.30
1	A	1434	ALA	CA-C-N	6.21	127.61	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1434	ALA	C-N-CA	6.21	127.61	119.84
3	C	106	GLU	N-CA-C	-6.20	106.04	113.97
7	I	75	CYS	CA-C-N	6.20	127.58	119.84
7	I	75	CYS	C-N-CA	6.20	127.58	119.84
3	C	211	ASP	CA-C-N	6.16	126.72	120.38
3	C	211	ASP	C-N-CA	6.16	126.72	120.38
6	H	109	LYS	CA-C-N	6.15	132.78	121.70
6	H	109	LYS	C-N-CA	6.15	132.78	121.70
2	B	276	ILE	N-CA-C	6.12	116.72	110.05
9	K	82	ASP	CA-C-N	6.08	126.52	119.47
9	K	82	ASP	C-N-CA	6.08	126.52	119.47
1	A	286	HIS	N-CA-C	6.02	118.37	111.02
1	A	483	ASP	N-CA-C	-5.98	103.69	111.71
1	A	864	ILE	N-CA-C	-5.98	106.66	111.81
7	I	31	THR	N-CA-C	-5.97	106.03	113.55
1	A	244	PRO	N-CA-C	5.90	117.89	110.70
1	A	513	SER	CA-C-N	5.85	126.26	119.47
1	A	513	SER	C-N-CA	5.85	126.26	119.47
2	B	470	LYS	N-CA-C	5.80	117.40	111.14
4	E	115	ASN	N-CA-C	5.78	115.73	108.45
2	B	801	LYS	CA-C-N	-5.70	113.83	119.92
2	B	801	LYS	C-N-CA	-5.70	113.83	119.92
2	B	1045	SER	CA-C-N	5.69	126.95	119.84
2	B	1045	SER	C-N-CA	5.69	126.95	119.84
4	E	164	LEU	N-CA-C	-5.60	105.09	111.14
1	A	241	VAL	N-CA-C	5.60	113.09	107.55
12	T	28	DC	O5'-C5'-C4'	5.58	119.16	110.80
1	A	466	SER	N-CA-C	5.55	119.75	113.15
1	A	267	ALA	N-CA-C	-5.54	106.45	113.43
2	B	273	LEU	CA-C-N	5.53	125.84	119.92
2	B	273	LEU	C-N-CA	5.53	125.84	119.92
1	A	227	VAL	N-CA-C	5.53	116.31	110.72
5	F	104	ASN	N-CA-C	5.50	122.51	110.80
2	B	1013	ASN	CA-C-N	5.49	126.70	119.84
2	B	1013	ASN	C-N-CA	5.49	126.70	119.84
1	A	55	ASP	N-CA-C	5.48	121.92	109.81
8	J	5	VAL	N-CA-C	-5.46	102.53	109.80
2	B	296	GLU	N-CA-C	-5.38	105.45	112.23
8	J	5	VAL	CB-CA-C	-5.38	103.85	111.28
2	B	1033	LYS	N-CA-C	-5.35	104.50	111.02
7	I	28	GLU	N-CA-C	5.33	116.24	108.14
1	A	746	MET	N-CA-C	-5.32	105.93	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	5	A	C5'-C4'-C3'	-5.30	108.05	116.00
7	I	70	ARG	N-CA-C	5.29	117.03	108.41
1	A	398	GLU	N-CA-C	-5.24	101.17	109.76
1	A	236	LEU	N-CA-C	5.23	117.28	108.96
2	B	1113	VAL	CB-CA-C	-5.21	105.22	112.04
1	A	1377	THR	N-CA-C	5.19	117.68	111.71
7	I	68	LEU	CA-C-N	5.17	125.62	120.14
7	I	68	LEU	C-N-CA	5.17	125.62	120.14
10	L	59	ALA	CB-CA-C	-5.16	110.21	117.23
2	B	973	ILE	CA-C-N	5.14	126.27	119.84
2	B	973	ILE	C-N-CA	5.14	126.27	119.84
2	B	816	GLU	N-CA-C	-5.13	108.77	114.62
1	A	1291	VAL	CA-C-N	5.12	125.41	119.93
1	A	1291	VAL	C-N-CA	5.12	125.41	119.93
10	L	55	ILE	N-CA-C	5.08	115.75	110.82
6	H	99	GLY	N-CA-C	5.08	118.68	111.12
4	E	168	TYR	N-CA-C	-5.07	106.00	113.61
2	B	744	HIS	CA-C-N	-5.07	114.44	119.56
2	B	744	HIS	C-N-CA	-5.07	114.44	119.56
2	B	37	PHE	N-CA-C	-5.07	103.79	110.43
1	A	1282	VAL	N-CA-C	5.02	115.14	108.27
1	A	845	LEU	N-CA-C	-5.01	107.72	113.88
3	C	183	TRP	N-CA-C	-5.01	102.87	110.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1172	LEU	Peptide
1	A	320	ARG	Peptide
2	B	473	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	10969	0	11070	759	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8792	0	8823	689	0
3	C	2095	0	2052	149	0
4	E	1752	0	1776	84	0
5	F	679	0	701	33	0
6	H	1068	0	1040	79	0
7	I	971	0	930	60	0
8	J	532	0	544	65	0
9	K	919	0	929	47	0
10	L	363	0	387	19	0
11	R	243	0	121	26	0
12	T	234	0	137	20	0
13	A	2	0	0	1	0
13	B	1	0	0	1	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	1	0
13	L	1	0	0	0	0
All	All	28625	0	28510	1808	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 32.

All (1808) 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)
2:B:778:MET:HE1	2:B:1094:ARG:NH1	1.40	1.35
2:B:704:ALA:HB1	2:B:710:LEU:CD1	1.55	1.34
2:B:634:TYR:HE1	2:B:692:TYR:CD1	1.51	1.28
2:B:634:TYR:CE1	2:B:692:TYR:HD1	1.52	1.27
2:B:879:ARG:CB	2:B:880:THR:HA	1.68	1.22
7:I:75:CYS:SG	7:I:78:CYS:HB2	1.82	1.19
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.26	1.14
1:A:1025:ARG:HG2	1:A:1025:ARG:HH11	1.04	1.14
2:B:879:ARG:HB2	2:B:880:THR:HA	1.20	1.14
1:A:565:ILE:HG23	1:A:567:LYS:HE3	1.31	1.12
8:J:43:ARG:HG3	8:J:46:CYS:HB2	1.32	1.11
2:B:222:ILE:HA	2:B:223:VAL:HB	1.17	1.11
2:B:464:GLY:HA3	2:B:478:GLY:HA2	1.32	1.10
2:B:1106:ARG:HD3	2:B:1126:GLY:O	1.53	1.09
1:A:899:VAL:CG1	1:A:929:LEU:HD13	1.84	1.08
2:B:636:PRO:HB2	2:B:637:LEU:HA	1.13	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:THR:HB	1:A:810:PRO:CD	1.84	1.07
1:A:630:ILE:H	1:A:630:ILE:HD12	1.20	1.06
2:B:955:THR:HG22	2:B:956:THR:H	1.15	1.06
1:A:899:VAL:HG13	1:A:929:LEU:HD13	1.09	1.06
2:B:704:ALA:CB	2:B:710:LEU:HD12	1.85	1.06
2:B:203:PHE:HE1	2:B:212:LEU:HD12	1.18	1.05
2:B:778:MET:HE1	2:B:1094:ARG:HH11	0.93	1.04
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.08	1.04
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.33	1.04
1:A:1323:ASP:OD2	1:A:1326:ARG:HG3	1.56	1.03
2:B:549:THR:HG22	2:B:550:ASP:H	1.24	1.03
2:B:636:PRO:HB2	2:B:637:LEU:CA	1.89	1.03
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.39	1.02
2:B:704:ALA:CB	2:B:710:LEU:CD1	2.37	1.01
2:B:778:MET:CE	2:B:1094:ARG:HH11	1.73	1.00
1:A:308:ILE:HG22	1:A:309:ALA:H	1.23	1.00
1:A:567:LYS:CG	1:A:568:PRO:HD2	1.90	1.00
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.42	1.00
1:A:567:LYS:HB3	6:H:96:VAL:H	1.26	1.00
1:A:264:PHE:HE1	1:A:317:LYS:HB2	1.23	0.99
1:A:1407:GLU:CD	1:A:1407:GLU:H	1.65	0.99
2:B:879:ARG:HB2	2:B:880:THR:CA	1.93	0.98
2:B:635:ARG:HB2	2:B:636:PRO:CD	1.95	0.97
2:B:902:GLY:O	2:B:903:VAL:O	1.83	0.97
2:B:635:ARG:CB	2:B:636:PRO:HD2	1.93	0.96
1:A:1284:MET:HB3	1:A:1306:LEU:HD23	1.44	0.96
1:A:827:THR:HG21	11:R:11:G:C4	1.99	0.95
8:J:10:CYS:SG	8:J:43:ARG:HD2	2.06	0.95
2:B:636:PRO:CB	2:B:637:LEU:HA	1.96	0.95
1:A:765:VAL:CG2	1:A:800:VAL:HB	1.96	0.94
2:B:1072:MET:HE2	2:B:1085:ILE:HG21	1.49	0.94
2:B:550:ASP:OD1	2:B:551:PRO:HD2	1.67	0.93
2:B:203:PHE:CE1	2:B:212:LEU:HD12	2.04	0.93
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.98	0.92
4:E:46:TYR:HE2	4:E:58:MET:HA	1.32	0.92
1:A:405:VAL:HG23	1:A:415:LEU:HD11	1.52	0.92
3:C:97:VAL:HG21	3:C:129:ILE:HG21	1.51	0.92
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.52	0.92
3:C:75:MET:HE1	3:C:239:PRO:HG3	1.53	0.91
1:A:873:MET:HE3	1:A:957:PRO:HG2	1.53	0.91
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.00	0.91
7:I:10:CYS:HB2	7:I:31:THR:OG1	1.70	0.91
2:B:567:GLU:H	2:B:567:GLU:CD	1.77	0.91
2:B:222:ILE:CA	2:B:223:VAL:HB	2.01	0.90
1:A:407:ARG:HD3	1:A:413:ILE:HD11	1.51	0.90
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.52	0.89
2:B:704:ALA:HB1	2:B:710:LEU:HD12	0.90	0.89
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.88	0.89
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.52	0.88
5:F:146:TRP:HB3	5:F:151:LEU:HD11	1.53	0.88
1:A:1025:ARG:HG2	1:A:1025:ARG:NH1	1.81	0.88
4:E:46:TYR:CE2	4:E:58:MET:HA	2.08	0.88
8:J:45:CYS:SG	8:J:46:CYS:N	2.46	0.88
4:E:14:ARG:HH12	4:E:142:VAL:HG22	1.38	0.87
12:T:27:DT:H2'	12:T:28:DC:H5''	1.54	0.87
1:A:1352:VAL:O	1:A:1355:VAL:HG12	1.75	0.87
2:B:464:GLY:HA3	2:B:478:GLY:CA	2.06	0.86
1:A:648:ASN:O	1:A:652:VAL:HG23	1.75	0.86
2:B:169:ARG:CG	2:B:169:ARG:HH11	1.88	0.86
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.54	0.86
8:J:8:PHE:H	8:J:49:MET:HE3	1.39	0.86
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.06	0.86
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.56	0.86
4:E:77:SER:HB3	4:E:105:PHE:HD2	1.40	0.86
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.58	0.86
1:A:809:THR:HB	1:A:810:PRO:HD3	1.57	0.85
2:B:600:LEU:HB3	2:B:615:MET:HE3	1.57	0.85
2:B:879:ARG:HB3	2:B:880:THR:HA	1.58	0.84
1:A:351:THR:HG22	1:A:352:VAL:N	1.91	0.84
7:I:73:ARG:O	7:I:81:ARG:HG2	1.77	0.84
1:A:535:THR:HG21	1:A:617:VAL:H	1.42	0.84
2:B:248:SER:H	2:B:418:LYS:HZ2	1.21	0.84
2:B:706:GLN:O	2:B:710:LEU:HB2	1.77	0.84
3:C:120:ILE:HG21	3:C:124:LEU:HD21	1.60	0.84
3:C:123:ASN:ND2	3:C:125:MET:HG2	1.93	0.83
1:A:315:LEU:CB	1:A:316:GLN:HA	2.07	0.83
1:A:264:PHE:CE1	1:A:317:LYS:HB2	2.13	0.83
4:E:28:TYR:CE1	4:E:78:LEU:HD13	2.13	0.83
1:A:1394:THR:HG21	1:A:1398:MET:HE3	1.60	0.83
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.42	0.83
2:B:986:GLN:NE2	2:B:1022:THR:HG21	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1163:CYS:HB3	2:B:1167:GLY:H	1.44	0.83
1:A:780:VAL:HG22	2:B:699:GLU:OE2	1.79	0.82
1:A:14:VAL:HG11	1:A:1430:LEU:HD13	1.60	0.82
2:B:911:ILE:CG2	2:B:966:VAL:HG11	2.08	0.82
2:B:473:MET:HA	2:B:474:SER:CB	2.08	0.82
1:A:1404:GLU:O	1:A:1408:ILE:HG12	1.80	0.82
2:B:955:THR:HG22	2:B:956:THR:N	1.91	0.82
1:A:1256:GLU:C	1:A:1258:HIS:H	1.88	0.82
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.62	0.82
1:A:304:MET:HG2	2:B:1210:MET:HG3	1.62	0.81
3:C:167:HIS:CD2	3:C:169:LYS:H	1.98	0.81
1:A:148:CYS:HB3	1:A:168:GLY:HA2	1.63	0.81
2:B:62:ILE:HD12	2:B:418:LYS:HG3	1.61	0.81
2:B:169:ARG:HH11	2:B:169:ARG:HG3	1.44	0.80
4:E:198:ILE:HD11	4:E:212:ARG:HG2	1.62	0.80
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.63	0.80
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	1.64	0.80
1:A:573:SER:O	1:A:576:GLN:HB2	1.81	0.80
2:B:955:THR:CG2	2:B:956:THR:H	1.95	0.80
1:A:567:LYS:CB	1:A:568:PRO:CD	2.59	0.80
2:B:707:PRO:HB3	2:B:741:CYS:SG	2.22	0.80
1:A:445:ASN:HB2	1:A:454:SER:O	1.80	0.79
2:B:216:GLU:HB3	2:B:500:THR:HG23	1.64	0.79
10:L:46:VAL:HG22	10:L:47:ARG:H	1.47	0.79
11:R:2:U:H2'	11:R:3:C:H6	1.47	0.79
1:A:455:MET:HE3	2:B:1134:GLU:HB3	1.65	0.79
1:A:315:LEU:HB2	1:A:316:GLN:HA	1.65	0.79
1:A:518:LYS:HG2	1:A:519:PRO:HD2	1.64	0.79
1:A:827:THR:HB	11:R:11:G:N3	1.97	0.79
2:B:37:PHE:O	2:B:38:PHE:HB2	1.83	0.78
2:B:796:LEU:CB	2:B:799:PRO:HG3	2.13	0.78
2:B:996:ARG:HG3	2:B:1007:VAL:HG21	1.63	0.78
1:A:43:GLU:HG3	1:A:46:THR:HB	1.65	0.78
1:A:820:GLY:O	1:A:821:ARG:HB3	1.83	0.78
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.66	0.78
1:A:829:VAL:C	1:A:831:THR:H	1.90	0.78
2:B:634:TYR:CE1	2:B:692:TYR:CD1	2.41	0.78
3:C:123:ASN:HD22	3:C:125:MET:CG	1.96	0.78
1:A:1004:ASN:OD1	1:A:1006:ILE:HD13	1.84	0.78
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.19	0.78
2:B:999:MET:HG2	2:B:1007:VAL:HG13	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:104:PHE:HD2	6:H:114:VAL:HG12	1.49	0.78
2:B:223:VAL:O	2:B:223:VAL:HG12	1.83	0.77
7:I:10:CYS:CB	7:I:31:THR:OG1	2.31	0.77
3:C:167:HIS:HD2	3:C:169:LYS:H	1.32	0.77
1:A:853:ASP:OD2	1:A:855:THR:HG22	1.85	0.77
1:A:335:ARG:HH11	2:B:1202:LEU:HD12	1.49	0.77
2:B:222:ILE:HA	2:B:223:VAL:CB	2.09	0.77
1:A:164:ARG:HG3	1:A:165:GLY:H	1.50	0.77
1:A:56:PRO:O	1:A:57:ARG:HG3	1.86	0.76
1:A:351:THR:CG2	1:A:352:VAL:N	2.47	0.76
2:B:464:GLY:CA	2:B:478:GLY:HA2	2.13	0.76
2:B:34:ILE:HG12	2:B:542:MET:HE3	1.66	0.76
4:E:198:ILE:HD11	4:E:212:ARG:CG	2.15	0.76
1:A:1029:ARG:HE	1:A:1033:GLN:HE22	1.32	0.76
2:B:956:THR:HA	2:B:961:LEU:O	1.84	0.76
3:C:123:ASN:ND2	3:C:125:MET:CG	2.48	0.76
7:I:63:GLY:HA3	7:I:104:LEU:HD11	1.66	0.76
1:A:809:THR:HG21	2:B:730:ARG:HG3	1.66	0.76
1:A:630:ILE:H	1:A:630:ILE:CD1	1.96	0.76
1:A:503:GLN:O	1:A:509:LEU:HD11	1.87	0.75
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.68	0.75
1:A:465:TYR:HB3	2:B:976:ILE:HG21	1.68	0.75
2:B:995:ARG:HG2	2:B:997:GLU:OE2	1.87	0.75
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.51	0.75
2:B:541:LEU:HD21	2:B:812:LEU:HD21	1.67	0.75
2:B:778:MET:CE	2:B:1094:ARG:NH1	2.35	0.75
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.27	0.75
1:A:451:HIS:HB2	1:A:453:MET:H	1.50	0.75
1:A:996:ASN:HA	1:A:998:LEU:HD23	1.69	0.75
11:R:2:U:H2'	11:R:3:C:C6	2.21	0.75
1:A:403:LYS:O	1:A:404:TYR:HB2	1.87	0.75
1:A:446:ARG:HB2	1:A:487:MET:HE2	1.68	0.75
3:C:97:VAL:HG21	3:C:129:ILE:CG2	2.17	0.75
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.65	0.74
2:B:515:HIS:H	2:B:518:HIS:HD2	1.34	0.74
6:H:84:ALA:C	6:H:86:ASP:H	1.91	0.74
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.69	0.74
1:A:809:THR:HB	1:A:810:PRO:HD2	1.66	0.74
2:B:1138:MET:HA	2:B:1138:MET:HE3	1.68	0.74
2:B:211:VAL:O	2:B:480:SER:HA	1.87	0.74
3:C:20:PHE:HD1	3:C:21:ILE:O	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ARG:O	1:A:825:ILE:HG12	1.88	0.74
3:C:123:ASN:HD22	3:C:125:MET:HG3	1.51	0.74
2:B:901:PRO:HG2	10:L:58:LYS:O	1.88	0.74
1:A:870:GLU:HB3	4:E:204:THR:CG2	2.18	0.73
2:B:473:MET:HA	2:B:474:SER:HB3	1.69	0.73
2:B:476:ARG:C	2:B:478:GLY:H	1.96	0.73
1:A:402:ALA:HB1	1:A:433:GLU:O	1.88	0.73
1:A:565:ILE:HG23	1:A:567:LYS:CE	2.14	0.73
2:B:179:CYS:SG	2:B:181:LEU:HD13	2.27	0.73
1:A:453:MET:C	1:A:455:MET:H	1.96	0.73
1:A:775:ILE:HG13	1:A:798:GLY:HA3	1.70	0.73
2:B:481:GLN:HB2	2:B:494:HIS:HE1	1.54	0.73
2:B:487:THR:O	2:B:488:TYR:C	2.31	0.73
1:A:401:GLY:C	1:A:435:HIS:CD2	2.67	0.73
1:A:858:ASN:C	1:A:858:ASN:HD22	1.96	0.73
2:B:223:VAL:O	2:B:223:VAL:CG1	2.37	0.73
1:A:99:ILE:HD13	1:A:235:ILE:HG23	1.69	0.73
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.71	0.73
1:A:575:LYS:HB3	1:A:612:ILE:HD11	1.71	0.73
2:B:474:SER:O	2:B:476:ARG:N	2.21	0.72
3:C:23:SER:O	3:C:25:VAL:HG23	1.89	0.72
6:H:24:CYS:HB2	6:H:44:VAL:HG23	1.69	0.72
2:B:957:ASN:HB3	2:B:961:LEU:HD12	1.71	0.72
3:C:54:ASN:HD22	3:C:54:ASN:C	1.97	0.72
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.24	0.72
2:B:169:ARG:HG3	2:B:169:ARG:NH1	2.03	0.72
8:J:43:ARG:HG3	8:J:46:CYS:CB	2.16	0.72
2:B:862:GLN:HE21	2:B:961:LEU:HD13	1.54	0.72
1:A:34:LYS:HD3	1:A:36:ARG:HH22	1.55	0.72
9:K:63:VAL:HG23	9:K:63:VAL:O	1.89	0.72
1:A:1156:PRO:HA	1:A:1190:PRO:HB3	1.72	0.72
2:B:125:SER:HA	2:B:171:PRO:HA	1.72	0.72
3:C:51:VAL:HA	3:C:155:LEU:HB3	1.72	0.71
1:A:645:LEU:HG	1:A:649:ILE:HD11	1.72	0.71
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.90	0.71
2:B:879:ARG:CB	2:B:880:THR:CA	2.54	0.71
2:B:999:MET:HA	2:B:999:MET:HE3	1.70	0.71
2:B:1051:THR:HB	2:B:1054:GLY:H	1.56	0.71
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.26	0.71
2:B:610:ASN:O	2:B:613:VAL:HG23	1.90	0.71
3:C:142:VAL:H	8:J:16:ASP:HB3	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:THR:HG21	11:R:11:G:N9	2.06	0.71
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.26	0.70
2:B:875:GLU:O	2:B:877:PRO:HD3	1.91	0.70
2:B:1056:SER:HB3	2:B:1066:SER:O	1.91	0.70
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.71	0.70
2:B:983:ARG:CD	2:B:1091:TYR:HB3	2.20	0.70
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.57	0.70
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.55	0.70
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.71	0.70
1:A:820:GLY:O	1:A:821:ARG:CB	2.40	0.70
1:A:1025:ARG:HH11	1:A:1025:ARG:CG	1.95	0.70
1:A:15:LYS:HE2	2:B:1220:ARG:HG2	1.73	0.70
2:B:46:GLN:NE2	2:B:496:ARG:HG2	2.06	0.70
1:A:896:ARG:HD2	1:A:897:TYR:CE1	2.27	0.70
1:A:55:ASP:O	1:A:58:LEU:N	2.25	0.70
2:B:203:PHE:CE1	2:B:212:LEU:CD1	2.73	0.70
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.23	0.70
1:A:858:ASN:HD22	1:A:860:LEU:H	1.40	0.70
6:H:91:ASP:C	6:H:93:TYR:H	2.00	0.70
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.73	0.69
2:B:549:THR:HG22	2:B:550:ASP:N	2.04	0.69
8:J:41:LEU:HD22	8:J:46:CYS:O	1.92	0.69
5:F:93:ILE:HD11	5:F:134:ILE:CD1	2.21	0.69
7:I:75:CYS:SG	7:I:78:CYS:CB	2.74	0.69
8:J:8:PHE:N	8:J:49:MET:HE3	2.08	0.69
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.73	0.69
1:A:53:LEU:HG	1:A:54:ASN:HD22	1.56	0.69
1:A:265:LYS:HD3	1:A:302:THR:HG22	1.74	0.69
2:B:1084:GLN:NE2	3:C:192:TRP:H	1.90	0.69
1:A:304:MET:CG	2:B:1210:MET:HG3	2.22	0.69
1:A:834:THR:HG21	1:A:1077:THR:HA	1.74	0.69
2:B:225:VAL:HG11	2:B:385:LEU:HA	1.74	0.69
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.75	0.69
2:B:704:ALA:HB2	2:B:738:PHE:CE2	2.27	0.69
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.57	0.69
8:J:43:ARG:CG	8:J:46:CYS:HB2	2.16	0.69
6:H:82:PRO:C	6:H:84:ALA:H	2.00	0.69
1:A:868:TYR:CE2	1:A:1366:ARG:HD3	2.28	0.69
1:A:886:ILE:CD1	1:A:943:LEU:HB3	2.21	0.68
1:A:77:CYS:SG	13:A:1735:ZN:ZN	1.83	0.68
1:A:511:ILE:HD13	1:A:646:PHE:HE1	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:109:LYS:HB3	6:H:110:ASP:CG	2.19	0.68
2:B:744:HIS:HD2	2:B:746:SER:H	1.41	0.68
1:A:253:ASN:CG	1:A:254:GLU:H	2.01	0.68
1:A:308:ILE:HG22	1:A:309:ALA:N	2.03	0.68
1:A:508:PRO:HB3	1:A:643:ALA:HB2	1.75	0.68
1:A:565:ILE:HG12	1:A:567:LYS:HZ1	1.56	0.68
3:C:35:ARG:HD3	9:K:41:THR:HA	1.75	0.68
4:E:199:ILE:O	4:E:199:ILE:HG22	1.92	0.68
1:A:397:ASN:OD1	1:A:397:ASN:N	2.27	0.68
1:A:265:LYS:NZ	1:A:322:VAL:HG12	2.09	0.68
1:A:324:SER:O	1:A:325:ILE:HB	1.92	0.68
6:H:109:LYS:HD2	6:H:111:LEU:HD12	1.75	0.68
2:B:493:SER:HB3	2:B:497:ARG:HH21	1.57	0.68
1:A:1356:ILE:HG21	1:A:1363:VAL:HG23	1.76	0.68
2:B:902:GLY:O	2:B:903:VAL:C	2.37	0.67
6:H:24:CYS:HB2	6:H:44:VAL:CG2	2.24	0.67
8:J:57:ILE:HA	8:J:60:PHE:HD2	1.58	0.67
2:B:1175:LEU:O	2:B:1176:ASN:HB2	1.94	0.67
3:C:54:ASN:ND2	3:C:56:THR:OG1	2.27	0.67
10:L:61:THR:CG2	10:L:62:LYS:N	2.56	0.67
1:A:1076:ALA:HA	1:A:1079:MET:HE2	1.75	0.67
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.30	0.67
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.60	0.67
2:B:744:HIS:CD2	2:B:745:PRO:HD2	2.30	0.67
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.75	0.67
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.76	0.67
3:C:33:LEU:HD12	3:C:37:MET:HE2	1.77	0.67
7:I:68:LEU:HB3	7:I:84:VAL:CG2	2.25	0.67
2:B:979:LYS:HG2	2:B:1095:LEU:HD12	1.77	0.67
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.60	0.67
3:C:58:LEU:CD2	3:C:145:CYS:HB2	2.25	0.67
2:B:957:ASN:O	2:B:959:ASP:N	2.28	0.67
2:B:997:GLU:HG2	3:C:39:ALA:HB2	1.75	0.67
3:C:77:ILE:HD12	3:C:161:LYS:HE2	1.77	0.67
5:F:85:MET:HE1	5:F:148:VAL:HG13	1.77	0.67
2:B:1084:GLN:HE22	3:C:192:TRP:N	1.94	0.66
2:B:359:GLU:HA	2:B:362:PRO:HG3	1.77	0.66
1:A:886:ILE:HG22	1:A:887:GLY:N	2.09	0.66
4:E:156:LEU:HD11	4:E:195:VAL:HB	1.76	0.66
1:A:946:VAL:HG22	4:E:201:LYS:HG3	1.78	0.66
2:B:212:LEU:HD23	2:B:479:VAL:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:751:VAL:HG13	2:B:812:LEU:CD1	2.25	0.66
2:B:1129:ARG:HE	2:B:1131:GLY:HA3	1.61	0.66
6:H:128:ASN:C	6:H:130:ARG:H	2.04	0.66
1:A:265:LYS:C	1:A:267:ALA:H	2.04	0.66
1:A:369:SER:HB3	9:K:2:ASN:HD21	1.61	0.66
8:J:5:VAL:O	8:J:6:ARG:O	2.13	0.66
1:A:855:THR:HG21	1:A:857:ARG:HE	1.59	0.66
1:A:873:MET:HE3	1:A:957:PRO:CG	2.26	0.66
3:C:58:LEU:HD23	3:C:145:CYS:HB2	1.78	0.66
3:C:183:TRP:CD1	3:C:183:TRP:H	2.12	0.66
2:B:552:MET:HA	2:B:555:ILE:HB	1.78	0.65
2:B:639:ILE:HA	2:B:740:HIS:HB3	1.78	0.65
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.60	0.65
1:A:1407:GLU:CD	1:A:1407:GLU:N	2.47	0.65
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.79	0.65
9:K:42:LEU:HG	9:K:42:LEU:O	1.95	0.65
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.78	0.65
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.27	0.65
2:B:21:GLU:HA	2:B:656:GLY:CA	2.26	0.65
2:B:110:HIS:CE1	10:L:53:HIS:HE1	2.15	0.65
3:C:120:ILE:HG21	3:C:124:LEU:CD2	2.27	0.65
1:A:1286:LYS:HE2	1:A:1302:PRO:HB2	1.78	0.65
2:B:805:THR:HG21	2:B:815:ARG:HH21	1.62	0.65
1:A:93:VAL:O	1:A:96:ILE:HG22	1.97	0.65
1:A:13:THR:HG22	1:A:1432:GLN:NE2	2.12	0.65
1:A:809:THR:CB	1:A:810:PRO:HD3	2.27	0.65
1:A:827:THR:CB	11:R:11:G:N3	2.59	0.65
1:A:1238:ILE:HG22	1:A:1240:CYS:SG	2.37	0.65
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.79	0.65
2:B:1081:LEU:HD12	2:B:1085:ILE:HD11	1.79	0.65
9:K:47:ARG:HB3	9:K:47:ARG:HH11	1.62	0.65
1:A:554:PRO:HG2	1:A:555:ASP:OD1	1.97	0.65
1:A:1004:ASN:ND2	4:E:167:ARG:HD3	2.12	0.65
2:B:170:LEU:HD12	2:B:171:PRO:HD2	1.79	0.65
2:B:428:ILE:HD11	2:B:448:ILE:HD13	1.79	0.64
2:B:476:ARG:O	2:B:478:GLY:N	2.30	0.64
3:C:255:VAL:O	3:C:258:ILE:HG22	1.97	0.64
11:R:9:G:H1	12:T:19:DC:H42	1.45	0.64
1:A:369:SER:CB	9:K:2:ASN:HD21	2.10	0.64
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.62	0.64
2:B:983:ARG:HD2	2:B:1091:TYR:CD2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1072:MET:HB2	2:B:1085:ILE:HD12	1.78	0.64
1:A:1116:LEU:N	1:A:1308:THR:HG22	2.13	0.64
2:B:708:GLU:C	2:B:710:LEU:H	2.05	0.64
2:B:916:THR:HG23	2:B:935:ARG:HB3	1.77	0.64
6:H:14:GLU:O	6:H:26:ILE:HD12	1.97	0.64
9:K:21:ILE:HD12	9:K:33:ILE:HG12	1.78	0.64
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.78	0.64
2:B:64:CYS:HA	2:B:67:SER:HB2	1.80	0.64
2:B:202:TYR:CE1	2:B:209:GLU:HG2	2.32	0.64
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.78	0.64
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.62	0.64
2:B:803:LEU:H	2:B:822:ASN:HD21	1.44	0.64
1:A:532:ARG:HH22	1:A:745:GLN:HG2	1.62	0.64
1:A:899:VAL:HG13	1:A:929:LEU:CD1	2.04	0.64
2:B:1166:CYS:SG	13:B:1307:ZN:ZN	1.86	0.64
1:A:407:ARG:HD3	1:A:413:ILE:CD1	2.27	0.64
2:B:698:GLU:O	2:B:701:ILE:HD13	1.98	0.64
1:A:381:THR:HG22	1:A:382:PRO:HD2	1.80	0.64
1:A:853:ASP:OD2	1:A:855:THR:CG2	2.46	0.64
1:A:1100:ARG:HH12	1:A:1111:MET:HE2	1.63	0.64
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.79	0.63
1:A:552:TRP:NE1	1:A:655:PHE:CD1	2.66	0.63
2:B:363:HIS:O	2:B:364:ILE:HB	1.98	0.63
1:A:335:ARG:NH1	2:B:1202:LEU:HD12	2.13	0.63
1:A:709:THR:HG23	7:I:94:ASP:HA	1.80	0.63
2:B:797:TYR:CE1	2:B:854:LEU:HD23	2.33	0.63
5:F:111:LEU:HD13	5:F:111:LEU:H	1.64	0.63
1:A:964:ILE:HD11	1:A:1037:LEU:HD21	1.81	0.63
1:A:630:ILE:O	1:A:634:THR:OG1	2.16	0.63
2:B:751:VAL:HG13	2:B:812:LEU:HD11	1.79	0.63
3:C:167:HIS:HD2	3:C:168:ALA:N	1.96	0.63
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.45	0.63
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.81	0.63
1:A:452:LYS:O	2:B:1141:HIS:CE1	2.51	0.63
4:E:15:ALA:O	4:E:19:VAL:HG23	1.98	0.63
2:B:706:GLN:O	2:B:710:LEU:CB	2.46	0.63
2:B:984:HIS:CE1	2:B:1025:HIS:HA	2.34	0.63
4:E:185:ALA:HB1	4:E:190:LEU:HG	1.80	0.63
7:I:17:ARG:HG2	7:I:18:GLU:H	1.64	0.63
3:C:261:ALA:HA	3:C:264:GLN:HG3	1.81	0.63
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.38	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:481:GLN:HB2	2:B:494:HIS:CE1	2.33	0.62
2:B:977:GLY:HA3	2:B:1099:VAL:CG1	2.29	0.62
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.82	0.62
1:A:630:ILE:HD12	1:A:630:ILE:N	2.03	0.62
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.81	0.62
1:A:402:ALA:CB	1:A:434:ARG:HA	2.29	0.62
1:A:613:ILE:HG23	6:H:117:SER:HB2	1.80	0.62
1:A:1363:VAL:HB	1:A:1368:MET:HE3	1.80	0.62
2:B:110:HIS:CE1	10:L:53:HIS:CE1	2.88	0.62
2:B:1065:GLN:O	2:B:1067:ARG:N	2.32	0.62
2:B:808:ALA:C	2:B:810:GLU:H	2.07	0.62
2:B:815:ARG:HG3	2:B:816:GLU:OE1	1.99	0.62
3:C:167:HIS:CD2	3:C:168:ALA:N	2.67	0.62
8:J:10:CYS:SG	8:J:43:ARG:CD	2.86	0.62
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.81	0.62
1:A:1332:PHE:CD1	1:A:1348:LEU:HD13	2.35	0.62
3:C:33:LEU:CD1	3:C:37:MET:HE2	2.30	0.62
1:A:48:ALA:C	1:A:49:LYS:HG2	2.23	0.62
1:A:267:ALA:O	1:A:271:LYS:HB2	2.00	0.62
2:B:345:LYS:N	2:B:348:ARG:HE	1.96	0.62
2:B:704:ALA:HB2	2:B:738:PHE:CD2	2.35	0.62
2:B:1034:VAL:HG22	2:B:1059:LEU:HB3	1.80	0.62
2:B:1066:SER:O	2:B:1067:ARG:HD2	2.00	0.62
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.35	0.62
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.82	0.62
10:L:61:THR:HG22	10:L:62:LYS:N	2.15	0.62
2:B:21:GLU:HA	2:B:656:GLY:HA3	1.81	0.62
2:B:478:GLY:O	2:B:480:SER:N	2.30	0.62
2:B:978:ASP:HB2	2:B:980:PHE:CE1	2.35	0.62
2:B:999:MET:HG2	2:B:1008:PRO:HD2	1.80	0.62
2:B:476:ARG:C	2:B:478:GLY:N	2.53	0.62
1:A:827:THR:CG2	11:R:11:G:C4	2.79	0.62
2:B:100:PRO:HA	2:B:126:SER:HA	1.81	0.61
2:B:468:GLU:HG3	2:B:469:GLN:H	1.65	0.61
2:B:248:SER:O	2:B:249:ARG:HB2	2.00	0.61
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.81	0.61
1:A:500:GLU:OE1	2:B:1144:ALA:N	2.32	0.61
1:A:577:ILE:O	1:A:580:VAL:HB	2.01	0.61
6:H:5:LEU:HD22	6:H:133:ASN:O	2.00	0.61
2:B:843:GLN:N	2:B:994:TYR:O	2.31	0.61
3:C:235:VAL:HG21	8:J:6:ARG:NH2	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:128:ASN:O	6:H:130:ARG:N	2.33	0.61
7:I:34:TYR:HE2	7:I:36:GLU:HG3	1.66	0.61
2:B:808:ALA:O	2:B:810:GLU:N	2.32	0.61
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.66	0.61
2:B:175:ARG:HH11	2:B:175:ARG:HG3	1.66	0.61
6:H:61:SER:HB2	6:H:139:ASN:HB3	1.83	0.61
1:A:956:LEU:HD21	1:A:1017:LEU:HD22	1.81	0.61
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.48	0.61
2:B:474:SER:C	2:B:476:ARG:N	2.59	0.61
2:B:542:MET:HG3	2:B:747:MET:CE	2.30	0.61
1:A:401:GLY:C	1:A:435:HIS:HD2	2.09	0.61
1:A:596:THR:C	1:A:598:LEU:H	2.09	0.61
1:A:889:SER:HB2	1:A:892:ALA:HB3	1.83	0.61
2:B:293:PRO:O	2:B:297:ILE:HG12	2.00	0.61
2:B:459:TYR:CD2	2:B:459:TYR:O	2.54	0.61
2:B:766:ARG:HA	2:B:769:TYR:HD1	1.66	0.61
3:C:54:ASN:HD22	3:C:56:THR:H	1.48	0.61
7:I:7:CYS:SG	7:I:9:ASP:N	2.74	0.61
1:A:77:CYS:SG	1:A:80:HIS:CE1	2.94	0.60
1:A:862:ASN:OD1	4:E:174:GLN:HA	2.01	0.60
1:A:1436:ILE:O	1:A:1437:GLY:C	2.44	0.60
2:B:20:ASP:N	2:B:655:LYS:HZ3	1.99	0.60
2:B:492:LEU:HB3	2:B:751:VAL:HG11	1.82	0.60
5:F:111:LEU:H	5:F:111:LEU:CD1	2.13	0.60
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.84	0.60
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.29	0.60
3:C:18:VAL:HG23	3:C:240:VAL:HG22	1.83	0.60
1:A:315:LEU:HB3	1:A:316:GLN:HA	1.83	0.60
2:B:1084:GLN:H	2:B:1084:GLN:CD	2.09	0.60
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.83	0.60
1:A:666:ILE:HD11	2:B:1030:LEU:HD22	1.83	0.60
1:A:979:SER:OG	1:A:980:ASP:N	2.34	0.60
2:B:102:VAL:HG23	2:B:110:HIS:HB3	1.83	0.60
2:B:219:ALA:HB2	2:B:405:ARG:HG2	1.82	0.60
2:B:542:MET:HB3	2:B:636:PRO:HD3	1.83	0.60
6:H:40:LEU:HG	6:H:42:ILE:CD1	2.31	0.60
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.66	0.60
8:J:46:CYS:SG	13:J:101:ZN:ZN	1.89	0.60
1:A:1039:LYS:O	1:A:1043:ASP:HB2	2.01	0.60
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.00	0.60
2:B:315:LYS:O	2:B:319:GLU:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:104:PHE:CD2	6:H:114:VAL:HG12	2.34	0.60
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.36	0.60
2:B:613:VAL:HG13	2:B:628:THR:HB	1.84	0.60
2:B:638:PHE:CE2	2:B:653:VAL:HG21	2.37	0.60
2:B:1175:LEU:O	2:B:1176:ASN:CB	2.50	0.60
2:B:190:TYR:CE1	8:J:62:ARG:HG2	2.37	0.60
2:B:999:MET:CG	2:B:1008:PRO:HD2	2.32	0.60
2:B:1159:ARG:HD3	2:B:1193:GLN:CG	2.31	0.60
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.36	0.60
1:A:754:SER:N	1:A:757:ASN:HD22	2.00	0.60
2:B:449:ASN:O	2:B:451:LYS:N	2.35	0.60
2:B:451:LYS:HA	2:B:454:THR:HB	1.83	0.60
6:H:4:THR:HA	6:H:60:ALA:HA	1.84	0.60
2:B:900:ALA:O	2:B:901:PRO:C	2.44	0.59
2:B:952:VAL:HG12	2:B:953:LEU:N	2.16	0.59
3:C:69:LEU:O	8:J:6:ARG:HD2	2.01	0.59
3:C:145:CYS:HA	8:J:2:ILE:HD13	1.84	0.59
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.36	0.59
12:T:26:DA:H2''	12:T:27:DT:H5''	1.84	0.59
1:A:261:ASP:HB3	1:A:323:LYS:HG3	1.83	0.59
2:B:803:LEU:N	2:B:822:ASN:HD21	1.99	0.59
1:A:518:LYS:HG2	1:A:519:PRO:CD	2.31	0.59
3:C:245:VAL:HA	3:C:248:ILE:HD12	1.83	0.59
2:B:174:LEU:HD22	2:B:204:ILE:HD11	1.83	0.59
2:B:789:MET:HE2	2:B:965:LYS:HB3	1.85	0.59
1:A:598:LEU:HB3	6:H:25:ARG:HH12	1.66	0.59
2:B:459:TYR:CD2	2:B:459:TYR:C	2.81	0.59
2:B:470:LYS:O	2:B:471:LYS:HG3	2.02	0.59
2:B:901:PRO:CG	10:L:58:LYS:O	2.50	0.59
2:B:901:PRO:HB2	10:L:60:ARG:HA	1.84	0.59
3:C:77:ILE:CD1	3:C:161:LYS:HE2	2.32	0.59
1:A:868:TYR:HE2	1:A:1366:ARG:HD3	1.66	0.59
2:B:484:ASN:ND2	2:B:490:SER:HB2	2.17	0.59
1:A:1005:GLU:HG3	1:A:1009:ASN:ND2	2.18	0.59
2:B:638:PHE:O	2:B:740:HIS:HB2	2.03	0.59
2:B:1084:GLN:NE2	3:C:192:TRP:N	2.49	0.59
3:C:98:VAL:HG12	3:C:99:LEU:N	2.18	0.59
7:I:94:ASP:OD2	7:I:94:ASP:N	2.34	0.59
1:A:105:CYS:SG	1:A:138:ILE:HG22	2.42	0.59
1:A:350:ARG:HD3	1:A:488:ASN:OD1	2.02	0.59
1:A:848:ILE:HG13	1:A:858:ASN:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:PRO:HG2	2:B:234:ILE:HD13	1.84	0.59
2:B:684:LEU:HD22	2:B:689:LEU:HD12	1.85	0.59
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.37	0.59
1:A:576:GLN:HA	1:A:576:GLN:HE21	1.68	0.58
1:A:256:GLN:HA	1:A:257:ARG:HB3	1.83	0.58
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.32	0.58
2:B:130:VAL:HG12	2:B:131:ASP:N	2.18	0.58
4:E:168:TYR:O	4:E:169:ARG:HG2	2.03	0.58
2:B:1135:ARG:O	2:B:1139:ILE:HG13	2.03	0.58
2:B:230:ALA:HA	2:B:261:ARG:NH1	2.18	0.58
2:B:843:GLN:NE2	2:B:847:ASP:OD1	2.36	0.58
2:B:860:MET:SD	2:B:861:ASP:N	2.77	0.58
1:A:1155:ASP:OD1	1:A:1161:THR:HA	2.03	0.58
1:A:774:ARG:HH21	1:A:797:LYS:HB2	1.68	0.58
2:B:977:GLY:HA3	2:B:1099:VAL:HG13	1.84	0.58
1:A:596:THR:O	1:A:598:LEU:N	2.35	0.58
1:A:658:LEU:HD22	2:B:831:SER:HA	1.85	0.58
2:B:640:VAL:HG13	2:B:650:GLU:O	2.04	0.58
1:A:405:VAL:HG22	1:A:432:VAL:HG13	1.86	0.58
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.86	0.58
2:B:516:ASN:HD22	2:B:516:ASN:H	1.50	0.58
3:C:70:ILE:HD11	3:C:144:ILE:CD1	2.33	0.58
9:K:40:HIS:CE1	9:K:63:VAL:HG11	2.38	0.58
1:A:782:ARG:HB3	1:A:788:SER:O	2.04	0.58
2:B:34:ILE:HG12	2:B:542:MET:CE	2.34	0.58
9:K:82:ASP:OD2	9:K:84:LYS:HB2	2.03	0.58
1:A:827:THR:HB	11:R:11:G:C2	2.39	0.57
1:A:1386:ARG:HG2	1:A:1403:GLU:OE1	2.04	0.57
2:B:1187:ASN:HD21	2:B:1190:ASP:H	1.52	0.57
6:H:36:CYS:HB2	6:H:130:ARG:HH22	1.67	0.57
2:B:861:ASP:OD1	2:B:914:LYS:HE2	2.04	0.57
2:B:898:LEU:HB2	10:L:58:LYS:HE3	1.86	0.57
4:E:170:LEU:HD13	4:E:175:LEU:HD22	1.85	0.57
6:H:89:LEU:HB2	6:H:91:ASP:HB3	1.84	0.57
9:K:65:HIS:C	9:K:67:PHE:H	2.11	0.57
1:A:1156:PRO:O	1:A:1158:PRO:HD3	2.04	0.57
1:A:14:VAL:CG1	1:A:1430:LEU:HD13	2.32	0.57
1:A:540:PHE:HZ	6:H:121:LEU:HD21	1.69	0.57
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.86	0.57
4:E:90:VAL:H	4:E:120:ALA:HB2	1.68	0.57
1:A:605:MET:HE3	1:A:614:PHE:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:GLU:HB3	4:E:204:THR:HG21	1.85	0.57
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.86	0.57
2:B:1012:ILE:HG21	2:B:1092:TYR:OH	2.04	0.57
6:H:109:LYS:CD	6:H:111:LEU:HD12	2.34	0.57
1:A:211:PHE:HA	1:A:214:ILE:HG12	1.87	0.57
1:A:518:LYS:CG	1:A:519:PRO:HD2	2.35	0.57
1:A:802:ASN:ND2	2:B:729:ILE:H	2.02	0.57
1:A:1059:HIS:ND1	5:F:86:THR:HA	2.19	0.57
2:B:634:TYR:CD1	2:B:692:TYR:HB3	2.40	0.57
2:B:825:VAL:HG23	2:B:1010:LEU:HB3	1.84	0.57
6:H:139:ASN:O	6:H:140:ALA:HB2	2.05	0.57
1:A:567:LYS:HB2	1:A:568:PRO:HD3	1.84	0.57
1:A:738:LYS:HE2	3:C:194:GLU:HA	1.85	0.57
3:C:261:ALA:HA	3:C:264:GLN:CG	2.35	0.57
1:A:224:PHE:HZ	1:A:234:MET:CE	2.18	0.57
1:A:315:LEU:CB	1:A:316:GLN:CA	2.83	0.57
1:A:399:HIS:O	1:A:401:GLY:N	2.34	0.57
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.40	0.57
2:B:169:ARG:CG	2:B:169:ARG:NH1	2.56	0.57
1:A:802:ASN:HD21	2:B:729:ILE:N	2.03	0.57
5:F:146:TRP:HB3	5:F:151:LEU:CD1	2.32	0.57
6:H:96:VAL:HA	6:H:142:LEU:O	2.05	0.57
9:K:21:ILE:CD1	9:K:33:ILE:HG12	2.34	0.57
1:A:261:ASP:HB3	1:A:323:LYS:CG	2.35	0.56
1:A:579:SER:HB3	1:A:611:GLN:HA	1.86	0.56
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.87	0.56
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.18	0.56
1:A:1301:GLU:HG3	1:A:1301:GLU:O	2.05	0.56
2:B:821:GLN:HE22	2:B:851:PHE:H	1.53	0.56
6:H:82:PRO:O	6:H:83:GLN:HB2	2.04	0.56
1:A:335:ARG:O	1:A:339:ASN:HB2	2.05	0.56
1:A:1404:GLU:HB3	1:A:1407:GLU:HG2	1.86	0.56
8:J:45:CYS:O	8:J:48:ARG:HG3	2.05	0.56
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.31	0.56
1:A:265:LYS:HZ1	1:A:322:VAL:HG12	1.71	0.56
1:A:446:ARG:HB3	1:A:478:TYR:HB3	1.87	0.56
1:A:453:MET:C	1:A:455:MET:N	2.63	0.56
1:A:457:ALA:HB2	1:A:505:CYS:HB2	1.86	0.56
1:A:775:ILE:O	1:A:797:LYS:HE2	2.05	0.56
2:B:744:HIS:CD2	2:B:745:PRO:CD	2.88	0.56
2:B:886:LYS:HB2	2:B:890:TYR:OH	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:THR:HG21	3:C:145:CYS:SG	2.45	0.56
1:A:559:VAL:HG23	1:A:559:VAL:O	2.05	0.56
1:A:607:ILE:HG12	1:A:612:ILE:HG22	1.87	0.56
1:A:1140:HIS:HB3	1:A:1279:ILE:O	2.05	0.56
3:C:91:HIS:HB3	3:C:96:SER:OG	2.04	0.56
1:A:242:PRO:HD2	1:A:266:LEU:HD11	1.87	0.56
1:A:567:LYS:NZ	6:H:97:MET:HB3	2.20	0.56
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.70	0.56
1:A:784:LEU:HB3	1:A:786:HIS:HD2	1.70	0.56
1:A:1116:LEU:HB2	1:A:1308:THR:HG21	1.87	0.56
1:A:1202:MET:HE1	1:A:1212:VAL:HG21	1.87	0.56
2:B:557:PHE:C	2:B:557:PHE:CD2	2.84	0.56
2:B:857:ARG:NH2	12:T:24:DC:OP1	2.38	0.56
2:B:1037:LEU:O	8:J:47:ARG:NH1	2.38	0.56
1:A:1325:THR:O	4:E:148:GLU:HG3	2.06	0.56
1:A:1428:VAL:HG22	2:B:1147:LEU:HD21	1.86	0.56
1:A:1436:ILE:O	1:A:1439:GLY:N	2.38	0.56
2:B:200:GLY:HA2	2:B:202:TYR:HE2	1.69	0.56
2:B:803:LEU:HD11	2:B:1036:ALA:HB2	1.88	0.56
6:H:96:VAL:HG13	6:H:143:LEU:HG	1.86	0.56
1:A:378:GLU:OE1	1:A:434:ARG:NH1	2.38	0.56
1:A:466:SER:O	2:B:1103:ILE:HD12	2.04	0.56
1:A:658:LEU:CD2	2:B:831:SER:HA	2.36	0.56
3:C:91:HIS:CE1	3:C:158:VAL:HG11	2.40	0.56
3:C:134:ILE:HG23	3:C:141:GLY:H	1.71	0.56
4:E:77:SER:HB3	4:E:105:PHE:CD2	2.31	0.56
7:I:28:GLU:HB3	7:I:35:VAL:HG22	1.88	0.56
1:A:662:PHE:HZ	1:A:746:MET:SD	2.28	0.56
1:A:885:THR:OG1	1:A:1024:SER:HB3	2.05	0.56
1:A:1239:ARG:HH11	1:A:1239:ARG:HB3	1.70	0.56
3:C:145:CYS:HA	8:J:2:ILE:CD1	2.36	0.56
6:H:128:ASN:C	6:H:130:ARG:N	2.61	0.56
1:A:855:THR:HG21	1:A:857:ARG:NE	2.21	0.56
3:C:22:LEU:HD21	3:C:25:VAL:HG21	1.88	0.56
1:A:50:ILE:HG22	1:A:52:GLY:N	2.21	0.56
1:A:469:ARG:NH2	2:B:991:GLY:O	2.39	0.56
2:B:1106:ARG:CD	2:B:1126:GLY:O	2.41	0.56
2:B:1169:MET:HE1	2:B:1201:LYS:HG2	1.88	0.56
1:A:423:ASP:C	1:A:424:ILE:HG12	2.31	0.55
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.87	0.55
2:B:369:GLY:O	2:B:370:PHE:CD1	2.59	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:THR:CG2	2:B:550:ASP:H	2.07	0.55
1:A:1284:MET:HB3	1:A:1306:LEU:CD2	2.27	0.55
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.87	0.55
2:B:778:MET:HE1	2:B:1094:ARG:HH12	1.59	0.55
1:A:14:VAL:HB	1:A:1432:GLN:HE22	1.72	0.55
1:A:455:MET:CE	2:B:1134:GLU:HB3	2.34	0.55
1:A:983:ILE:O	1:A:983:ILE:HG22	2.07	0.55
3:C:129:ILE:HG23	3:C:130:GLY:N	2.22	0.55
10:L:60:ARG:HG3	10:L:61:THR:N	2.21	0.55
1:A:34:LYS:HD3	1:A:36:ARG:NH2	2.19	0.55
1:A:534:LEU:O	1:A:574:GLY:HA3	2.07	0.55
2:B:1034:VAL:CG2	2:B:1059:LEU:HB3	2.36	0.55
4:E:179:GLN:O	4:E:182:ASP:HB2	2.06	0.55
1:A:827:THR:HG21	11:R:11:G:O4'	2.06	0.55
1:A:1256:GLU:C	1:A:1258:HIS:N	2.57	0.55
1:A:1378:GLN:NE2	1:A:1392:SER:HB2	2.21	0.55
2:B:1001:PHE:CE2	2:B:1073:TYR:HB2	2.42	0.55
4:E:202:SER:HB3	4:E:205:SER:O	2.06	0.55
2:B:199:MET:N	2:B:199:MET:SD	2.80	0.55
2:B:261:ARG:N	2:B:264:SER:HB3	2.21	0.55
2:B:805:THR:OG1	2:B:815:ARG:NH2	2.40	0.55
2:B:37:PHE:O	2:B:38:PHE:CB	2.54	0.55
2:B:256:VAL:CG1	2:B:382:ILE:HD13	2.32	0.55
2:B:638:PHE:O	2:B:740:HIS:CB	2.55	0.55
2:B:803:LEU:HD21	8:J:51:LEU:HD23	1.89	0.55
6:H:84:ALA:C	6:H:86:ASP:N	2.59	0.55
7:I:46:HIS:HD1	7:I:46:HIS:C	2.15	0.55
7:I:119:THR:O	7:I:120:GLN:HB2	2.05	0.55
1:A:351:THR:HG21	1:A:466:SER:O	2.06	0.55
2:B:240:ILE:HG21	2:B:381:MET:HE2	1.88	0.55
6:H:91:ASP:C	6:H:93:TYR:N	2.64	0.55
7:I:92:ARG:HG2	7:I:93:LYS:H	1.72	0.55
2:B:711:GLU:N	2:B:712:PRO:HD3	2.22	0.55
4:E:161:LYS:HD2	4:E:195:VAL:HG23	1.89	0.55
1:A:472:LEU:HD13	2:B:835:GLN:NE2	2.22	0.55
1:A:504:LEU:HD12	1:A:504:LEU:N	2.22	0.55
2:B:481:GLN:OE1	2:B:494:HIS:NE2	2.39	0.55
2:B:704:ALA:CB	2:B:710:LEU:HD13	2.33	0.55
1:A:364:VAL:O	1:A:364:VAL:HG13	2.07	0.54
1:A:939:ASP:O	1:A:940:ARG:C	2.50	0.54
1:A:1351:GLU:O	1:A:1352:VAL:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ILE:HG13	2:B:542:MET:HE1	1.89	0.54
2:B:1074:ASN:HD22	2:B:1077:THR:H	1.55	0.54
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.88	0.54
1:A:588:LEU:HD23	1:A:605:MET:HG2	1.88	0.54
1:A:744:LYS:HE2	1:A:748:MET:HE3	1.89	0.54
1:A:999:VAL:HG23	1:A:1053:PHE:HE2	1.72	0.54
2:B:992:ILE:HD11	9:K:67:PHE:HE2	1.72	0.54
3:C:178:PHE:C	3:C:178:PHE:CD2	2.86	0.54
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.46	0.54
4:E:19:VAL:O	4:E:23:VAL:HG23	2.06	0.54
4:E:113:GLN:HA	4:E:137:GLU:HG3	1.88	0.54
7:I:40:SER:HB2	7:I:41:PRO:HD2	1.89	0.54
1:A:30:ILE:HG12	2:B:1170:THR:HG21	1.89	0.54
1:A:832:ALA:HB2	12:T:18:DT:H72	1.89	0.54
2:B:801:LYS:O	8:J:52:THR:CG2	2.55	0.54
2:B:1059:LEU:HG	2:B:1059:LEU:O	2.07	0.54
2:B:1154:ALA:O	2:B:1155:SER:HB3	2.07	0.54
3:C:54:ASN:ND2	3:C:56:THR:H	2.05	0.54
7:I:111:THR:HG22	7:I:113:ASP:H	1.73	0.54
1:A:572:TRP:N	1:A:572:TRP:CE3	2.75	0.54
1:A:890:ASP:HB2	1:A:1295:THR:O	2.08	0.54
2:B:487:THR:CG2	2:B:819:ALA:HB2	2.37	0.54
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.89	0.54
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.88	0.54
1:A:92:HIS:HB3	1:A:95:PHE:HB2	1.88	0.54
1:A:869:GLY:O	4:E:204:THR:HG21	2.08	0.54
1:A:1376:THR:CG2	4:E:212:ARG:HH22	2.20	0.54
2:B:1077:THR:CG2	2:B:1079:LYS:HB2	2.37	0.54
1:A:852:TYR:CE2	5:F:136:ARG:HG2	2.42	0.54
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.43	0.54
1:A:1005:GLU:HG3	1:A:1009:ASN:HD21	1.73	0.54
2:B:904:ARG:HG2	2:B:948:ILE:HG12	1.90	0.54
2:B:1024:ALA:O	2:B:1027:ILE:N	2.41	0.54
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.88	0.54
1:A:566:ILE:HG22	1:A:566:ILE:O	2.08	0.54
1:A:1100:ARG:O	1:A:1101:LEU:C	2.51	0.54
2:B:240:ILE:HG21	2:B:381:MET:CE	2.37	0.54
1:A:675:THR:HG21	1:A:736:ASN:HB2	1.90	0.54
1:A:910:PRO:HA	1:A:916:GLY:HA3	1.90	0.54
1:A:974:ASP:OD1	1:A:977:LYS:HB2	2.07	0.54
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:92:ARG:HG2	5:F:92:ARG:O	2.08	0.54
7:I:63:GLY:CA	7:I:104:LEU:HD11	2.37	0.54
1:A:1406:VAL:N	1:A:1407:GLU:OE2	2.40	0.54
2:B:210:LYS:HB3	2:B:480:SER:OG	2.08	0.54
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.42	0.54
2:B:911:ILE:HG21	2:B:966:VAL:HG11	1.87	0.54
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.08	0.54
1:A:827:THR:CG2	11:R:11:G:O4'	2.56	0.53
1:A:883:LEU:HB2	1:A:952:ALA:HB1	1.90	0.53
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.90	0.53
1:A:1436:ILE:CG2	1:A:1437:GLY:N	2.71	0.53
2:B:581:PHE:HA	2:B:585:VAL:O	2.08	0.53
2:B:1076:HIS:HB3	9:K:40:HIS:CD2	2.43	0.53
7:I:19:ASP:O	7:I:23:ASN:HA	2.08	0.53
1:A:527:THR:HG23	1:A:653:VAL:HG21	1.89	0.53
1:A:529:CYS:O	1:A:533:LYS:HG3	2.07	0.53
1:A:800:VAL:HG13	1:A:812:GLU:HB3	1.89	0.53
1:A:802:ASN:CG	2:B:729:ILE:H	2.16	0.53
1:A:993:LEU:HD21	1:A:1022:LEU:HD11	1.89	0.53
2:B:550:ASP:OD1	2:B:551:PRO:CD	2.49	0.53
1:A:482:PHE:HD1	2:B:835:GLN:O	1.91	0.53
1:A:1398:MET:O	1:A:1399:ARG:C	2.52	0.53
1:A:528:LEU:HA	1:A:531:ILE:HG22	1.89	0.53
1:A:567:LYS:HZ1	6:H:97:MET:HB3	1.72	0.53
1:A:858:ASN:C	1:A:858:ASN:ND2	2.64	0.53
4:E:32:GLN:HA	4:E:35:VAL:HG12	1.90	0.53
6:H:47:PHE:CB	6:H:95:TYR:HD1	2.21	0.53
2:B:46:GLN:HE21	2:B:496:ARG:HG2	1.74	0.53
2:B:98:THR:HG21	2:B:101:MET:HE2	1.89	0.53
2:B:696:GLU:O	2:B:699:GLU:HB2	2.08	0.53
3:C:98:VAL:CG1	3:C:99:LEU:N	2.71	0.53
4:E:61:GLN:HB2	4:E:79:TRP:HE3	1.72	0.53
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.88	0.53
11:R:8:G:H2'	11:R:9:G:C8	2.43	0.53
1:A:14:VAL:HG11	1:A:1430:LEU:CD1	2.36	0.53
1:A:265:LYS:O	1:A:267:ALA:N	2.42	0.53
2:B:369:GLY:O	2:B:370:PHE:HD1	1.91	0.53
2:B:701:ILE:HG21	2:B:740:HIS:HE1	1.73	0.53
2:B:1129:ARG:HE	2:B:1131:GLY:CA	2.20	0.53
1:A:565:ILE:CG2	1:A:567:LYS:HE3	2.22	0.53
1:A:942:PHE:C	1:A:942:PHE:CD2	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:808:ALA:O	2:B:812:LEU:HD23	2.09	0.53
3:C:43:THR:HG22	3:C:44:LEU:H	1.73	0.53
8:J:9:SER:OG	8:J:48:ARG:NH2	2.41	0.53
9:K:58:PHE:HE2	9:K:74:ARG:HE	1.57	0.53
1:A:650:GLN:O	1:A:654:ASN:HB2	2.08	0.53
2:B:174:LEU:CD2	2:B:204:ILE:HD11	2.39	0.53
2:B:546:SER:HB3	2:B:632:ARG:H	1.74	0.53
2:B:1033:LYS:NZ	2:B:1070:GLU:OE1	2.35	0.53
3:C:248:ILE:O	3:C:252:GLN:HB2	2.08	0.53
1:A:14:VAL:H	1:A:1432:GLN:NE2	2.06	0.53
1:A:1352:VAL:O	1:A:1355:VAL:CG1	2.53	0.53
2:B:792:MET:HE1	12:T:23:DT:O3'	2.09	0.53
4:E:10:SER:O	4:E:14:ARG:HG3	2.08	0.53
1:A:827:THR:CG2	11:R:11:G:N3	2.72	0.53
1:A:829:VAL:C	1:A:831:THR:N	2.62	0.53
1:A:858:ASN:ND2	1:A:860:LEU:H	2.07	0.53
2:B:708:GLU:O	2:B:710:LEU:N	2.42	0.53
2:B:722:ASP:OD2	2:B:723:VAL:HG23	2.09	0.53
3:C:123:ASN:HD21	3:C:125:MET:HG2	1.71	0.53
7:I:59:VAL:HG12	7:I:60:GLN:H	1.73	0.53
1:A:226:GLU:HG3	1:A:230:ARG:HH21	1.74	0.52
1:A:434:ARG:HE	1:A:437:MET:HG3	1.73	0.52
1:A:452:LYS:HB2	2:B:1141:HIS:CE1	2.44	0.52
2:B:634:TYR:HD1	2:B:692:TYR:HB3	1.74	0.52
7:I:25:LEU:HG	7:I:38:ALA:HB3	1.91	0.52
1:A:573:SER:H	1:A:576:GLN:HG3	1.75	0.52
2:B:175:ARG:HG3	2:B:175:ARG:NH1	2.23	0.52
3:C:18:VAL:CG2	3:C:240:VAL:HG22	2.39	0.52
3:C:40:GLU:OE1	3:C:254:LYS:NZ	2.35	0.52
2:B:880:THR:O	2:B:881:ASN:HB2	2.08	0.52
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.45	0.52
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.44	0.52
1:A:247:ARG:HG3	1:A:262:LEU:HB2	1.91	0.52
1:A:1427:ASN:HB2	1:A:1434:ALA:HB2	1.92	0.52
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.92	0.52
7:I:75:CYS:HB3	7:I:110:PHE:CE2	2.45	0.52
1:A:751:SER:HB2	2:B:1015:HIS:CE1	2.45	0.52
1:A:795:GLU:HB3	2:B:731:VAL:HG11	1.92	0.52
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.90	0.52
2:B:1027:ILE:O	2:B:1028:GLU:C	2.50	0.52
4:E:177:ARG:HD3	4:E:215:MET:SD	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:HIS:HB2	1:A:453:MET:N	2.23	0.52
1:A:899:VAL:HG13	1:A:899:VAL:O	2.09	0.52
2:B:306:ASN:O	2:B:308:TRP:N	2.43	0.52
3:C:141:GLY:HA2	8:J:16:ASP:HB3	1.91	0.52
3:C:165:LYS:O	9:K:6:ARG:NH1	2.41	0.52
8:J:24:LEU:O	8:J:30:LEU:HB2	2.08	0.52
8:J:36:LEU:HD11	8:J:51:LEU:HD13	1.90	0.52
11:R:9:G:H1	12:T:19:DC:N4	2.07	0.52
1:A:58:LEU:HD23	1:A:58:LEU:C	2.34	0.52
1:A:260:ASP:OD1	1:A:261:ASP:N	2.40	0.52
1:A:315:LEU:HB3	1:A:316:GLN:CA	2.39	0.52
1:A:351:THR:CG2	1:A:352:VAL:H	2.20	0.52
1:A:1341:ILE:HB	4:E:182:ASP:OD2	2.09	0.52
2:B:321:GLY:C	2:B:323:VAL:H	2.18	0.52
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.91	0.52
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.75	0.52
2:B:1056:SER:CB	2:B:1066:SER:O	2.57	0.52
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.25	0.52
9:K:46:ILE:O	9:K:50:LEU:N	2.42	0.52
1:A:51:GLY:HA2	1:A:56:PRO:HG3	1.92	0.52
1:A:1327:ILE:O	4:E:147:HIS:HE1	1.93	0.52
2:B:197:PHE:CG	2:B:817:LEU:HD11	2.45	0.52
2:B:823:ALA:HA	8:J:48:ARG:NH1	2.24	0.52
1:A:71:GLN:C	1:A:73:GLY:H	2.18	0.52
1:A:826:ASP:OD2	1:A:826:ASP:N	2.43	0.52
2:B:745:PRO:O	2:B:748:ILE:HG13	2.10	0.52
2:B:1034:VAL:HG22	2:B:1059:LEU:CB	2.40	0.52
2:B:1065:GLN:NE2	2:B:1067:ARG:H	2.07	0.52
1:A:58:LEU:HD21	1:A:244:PRO:HD2	1.92	0.52
1:A:65:LEU:O	1:A:71:GLN:HA	2.09	0.52
1:A:396:PRO:HB3	1:A:403:LYS:HB3	1.91	0.52
1:A:525:GLN:O	1:A:526:ASP:C	2.52	0.52
1:A:572:TRP:N	1:A:572:TRP:HE3	2.08	0.52
2:B:577:ALA:HB1	2:B:589:VAL:HG12	1.92	0.52
7:I:75:CYS:SG	7:I:103:CYS:SG	3.00	0.52
1:A:802:ASN:HD21	2:B:729:ILE:H	1.56	0.51
2:B:315:LYS:HG2	7:I:13:MET:HE1	1.92	0.51
3:C:9:LYS:O	3:C:20:PHE:HB2	2.10	0.51
1:A:353:ILE:CD1	1:A:487:MET:HE3	2.39	0.51
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.92	0.51
2:B:801:LYS:HG3	2:B:802:PRO:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:944:THR:HG21	2:B:1122:ARG:HH22	1.76	0.51
2:B:110:HIS:HE1	10:L:53:HIS:CE1	2.28	0.51
2:B:999:MET:HA	2:B:999:MET:CE	2.39	0.51
10:L:60:ARG:HG3	10:L:61:THR:H	1.74	0.51
1:A:457:ALA:O	1:A:507:VAL:HG23	2.10	0.51
1:A:1377:THR:HG22	4:E:176:PRO:HB3	1.92	0.51
1:A:1378:GLN:HE22	1:A:1392:SER:HB2	1.75	0.51
1:A:1419:ASP:OD1	1:A:1420:ASP:N	2.44	0.51
2:B:190:TYR:HD2	8:J:63:TYR:CE2	2.29	0.51
3:C:235:VAL:HG21	8:J:6:ARG:HH21	1.76	0.51
5:F:116:ASP:OD2	5:F:117:PRO:HD2	2.11	0.51
1:A:870:GLU:HB3	4:E:204:THR:HG23	1.92	0.51
2:B:474:SER:C	2:B:476:ARG:H	2.13	0.51
2:B:567:GLU:CD	2:B:567:GLU:N	2.56	0.51
2:B:723:VAL:O	2:B:724:ASP:C	2.54	0.51
1:A:332:LYS:H	1:A:337:ARG:HB3	1.75	0.51
1:A:567:LYS:HB3	6:H:96:VAL:N	2.10	0.51
1:A:827:THR:O	1:A:827:THR:HG22	2.10	0.51
1:A:889:SER:HB2	1:A:892:ALA:CB	2.41	0.51
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.10	0.51
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.25	0.51
2:B:483:LEU:HD22	2:B:491:THR:HG23	1.93	0.51
2:B:703:ILE:HA	2:B:740:HIS:O	2.10	0.51
1:A:998:LEU:CD1	1:A:1001:ARG:HG3	2.41	0.51
2:B:185:THR:OG1	2:B:188:ASP:HB2	2.11	0.51
2:B:364:ILE:O	2:B:365:THR:HB	2.11	0.51
9:K:102:LYS:O	9:K:106:GLU:HG2	2.11	0.51
1:A:472:LEU:O	1:A:475:THR:HB	2.10	0.51
2:B:102:VAL:HG11	2:B:122:LEU:HD13	1.93	0.51
2:B:173:MET:HE2	2:B:201:GLY:O	2.11	0.51
2:B:563:MET:HG3	2:B:563:MET:O	2.10	0.51
3:C:261:ALA:HA	3:C:264:GLN:HE21	1.74	0.51
6:H:36:CYS:HA	6:H:126:GLU:O	2.11	0.51
1:A:1428:VAL:HG13	2:B:1151:LEU:HD23	1.93	0.51
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.26	0.51
2:B:648:HIS:HD2	2:B:649:LYS:O	1.94	0.51
3:C:127:ARG:HG3	3:C:129:ILE:HD13	1.92	0.51
6:H:102:TYR:OH	6:H:122:LEU:HD22	2.11	0.51
1:A:329:LEU:HD13	1:A:335:ARG:HB3	1.93	0.51
2:B:975:GLN:NE2	2:B:1100:ASP:OD2	2.44	0.51
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:HIS:CD2	2:B:516:ASN:N	2.80	0.50
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.11	0.50
3:C:251:LEU:O	3:C:255:VAL:HG23	2.10	0.50
6:H:47:PHE:HB3	6:H:95:TYR:HD1	1.76	0.50
9:K:63:VAL:O	9:K:63:VAL:CG2	2.59	0.50
1:A:544:ASP:HB2	9:K:47:ARG:NH2	2.24	0.50
2:B:173:MET:O	2:B:176:SER:OG	2.29	0.50
12:T:23:DT:H2'	12:T:24:DC:H6	1.75	0.50
1:A:247:ARG:HG2	1:A:263:THR:OG1	2.11	0.50
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.47	0.50
1:A:563:PRO:HB2	1:A:565:ILE:O	2.11	0.50
1:A:667:GLY:HA2	1:A:670:ILE:CG1	2.41	0.50
1:A:1161:THR:HG23	1:A:1239:ARG:HH21	1.77	0.50
1:A:1394:THR:CG2	1:A:1398:MET:HE3	2.38	0.50
2:B:464:GLY:HA3	2:B:478:GLY:C	2.35	0.50
4:E:162:ARG:HA	4:E:165:LEU:HB2	1.93	0.50
1:A:308:ILE:CG2	1:A:309:ALA:H	2.05	0.50
1:A:939:ASP:OD2	1:A:1023:ARG:HD2	2.11	0.50
2:B:777:ALA:O	2:B:819:ALA:HB1	2.12	0.50
4:E:195:VAL:HG12	4:E:196:VAL:O	2.12	0.50
1:A:99:ILE:CD1	1:A:235:ILE:HG23	2.42	0.50
1:A:343:LYS:HZ2	2:B:1197:PRO:HB3	1.77	0.50
1:A:364:VAL:HG12	1:A:459:ARG:O	2.11	0.50
2:B:545:ILE:C	2:B:634:TYR:HE2	2.20	0.50
1:A:265:LYS:NZ	1:A:323:LYS:HG2	2.27	0.50
1:A:889:SER:HB2	1:A:892:ALA:H	1.75	0.50
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.76	0.50
2:B:981:ALA:HB3	2:B:1095:LEU:HD21	1.92	0.50
2:B:986:GLN:HE21	2:B:1022:THR:HG21	1.71	0.50
11:R:7:A:H61	12:T:21:DT:H3	1.60	0.50
1:A:666:ILE:CD1	2:B:1030:LEU:HD22	2.41	0.50
1:A:1213:GLY:HA3	1:A:1228:TRP:CZ3	2.46	0.50
2:B:213:ILE:O	2:B:215:GLN:OE1	2.30	0.50
2:B:490:SER:OG	2:B:491:THR:N	2.43	0.50
2:B:805:THR:CB	2:B:815:ARG:NH2	2.75	0.50
2:B:900:ALA:O	2:B:901:PRO:O	2.30	0.50
3:C:166:GLU:O	3:C:167:HIS:HB2	2.10	0.50
4:E:28:TYR:CD1	4:E:78:LEU:HD13	2.45	0.50
7:I:25:LEU:HD23	7:I:25:LEU:H	1.75	0.50
8:J:43:ARG:O	8:J:47:ARG:N	2.44	0.50
8:J:57:ILE:O	8:J:60:PHE:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:THR:HG21	1:A:313:GLN:OE1	2.11	0.50
1:A:1116:LEU:HD13	1:A:1329:THR:HG23	1.94	0.50
2:B:224:GLN:O	2:B:238:ALA:HA	2.12	0.50
2:B:806:THR:HG22	2:B:808:ALA:H	1.76	0.50
2:B:850:LEU:HD12	8:J:8:PHE:CD1	2.47	0.50
2:B:1076:HIS:H	2:B:1076:HIS:CD2	2.29	0.50
1:A:380:VAL:HG12	1:A:428:TYR:HA	1.94	0.50
1:A:567:LYS:HG3	1:A:568:PRO:CD	2.19	0.50
1:A:722:LEU:HD11	1:A:794:PRO:HB3	1.93	0.50
1:A:982:THR:C	1:A:984:LYS:N	2.70	0.50
1:A:1258:HIS:CD2	1:A:1262:LYS:HD2	2.47	0.50
2:B:1029:CYS:SG	2:B:1090:THR:OG1	2.68	0.50
4:E:127:ILE:HD13	4:E:127:ILE:N	2.27	0.50
1:A:456:MET:HG3	1:A:507:VAL:HG22	1.92	0.49
1:A:473:SER:O	1:A:521:MET:HB3	2.13	0.49
1:A:504:LEU:HD11	5:F:91:ALA:CB	2.40	0.49
1:A:845:LEU:HA	1:A:848:ILE:HD13	1.93	0.49
1:A:997:LEU:HD22	1:A:1053:PHE:CD1	2.47	0.49
2:B:698:GLU:HA	2:B:701:ILE:CD1	2.42	0.49
2:B:1164:GLY:HA3	2:B:1190:ASP:HB3	1.94	0.49
6:H:39:THR:OG1	6:H:124:ARG:HB3	2.12	0.49
6:H:109:LYS:HB3	6:H:110:ASP:C	2.37	0.49
8:J:23:ASN:C	8:J:25:LEU:H	2.20	0.49
1:A:50:ILE:HG22	1:A:52:GLY:H	1.77	0.49
1:A:909:ASP:OD2	1:A:910:PRO:HD2	2.13	0.49
1:A:1349:TYR:O	1:A:1350:LYS:C	2.55	0.49
2:B:487:THR:O	2:B:489:SER:N	2.45	0.49
2:B:730:ARG:HH11	2:B:730:ARG:HB2	1.77	0.49
2:B:821:GLN:H	2:B:851:PHE:HE2	1.60	0.49
2:B:968:VAL:HG12	2:B:969:ARG:N	2.27	0.49
3:C:33:LEU:HD12	3:C:37:MET:CE	2.41	0.49
3:C:196:ASP:C	3:C:198:ALA:H	2.21	0.49
1:A:330:LYS:O	1:A:334:GLY:HA3	2.12	0.49
1:A:367:PRO:HB3	1:A:466:SER:HA	1.94	0.49
1:A:727:ASP:O	1:A:731:ARG:HD3	2.13	0.49
3:C:123:ASN:ND2	3:C:125:MET:HG3	2.21	0.49
3:C:129:ILE:CG2	3:C:130:GLY:N	2.75	0.49
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.94	0.49
1:A:827:THR:HG21	11:R:11:G:N3	2.26	0.49
2:B:487:THR:HG21	2:B:819:ALA:HB2	1.93	0.49
2:B:882:THR:HG23	2:B:884:ARG:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:910:VAL:HG12	2:B:911:ILE:N	2.27	0.49
3:C:29:MET:O	3:C:30:ALA:C	2.54	0.49
1:A:134:ARG:HD3	1:A:221:SER:O	2.13	0.49
1:A:704:ALA:HB2	1:A:710:LEU:HG	1.94	0.49
1:A:1116:LEU:H	1:A:1308:THR:CG2	2.23	0.49
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.94	0.49
2:B:186:GLU:O	2:B:187:SER:C	2.56	0.49
4:E:190:LEU:HD12	4:E:214:CYS:HB2	1.95	0.49
1:A:27:VAL:O	1:A:30:ILE:HG22	2.12	0.49
1:A:456:MET:CG	1:A:478:TYR:OH	2.60	0.49
1:A:1376:THR:HG22	4:E:212:ARG:HH22	1.78	0.49
1:A:1406:VAL:HA	1:A:1409:LEU:HD12	1.94	0.49
2:B:482:VAL:O	2:B:483:LEU:C	2.54	0.49
2:B:708:GLU:OE2	2:B:709:ASP:HB2	2.11	0.49
2:B:862:GLN:NE2	2:B:961:LEU:HD13	2.25	0.49
6:H:145:ARG:HG3	6:H:146:ARG:HG2	1.95	0.49
8:J:25:LEU:HD21	8:J:32:GLU:HA	1.95	0.49
1:A:472:LEU:HD22	2:B:835:GLN:HB2	1.94	0.49
1:A:760:GLN:HA	1:A:764:CYS:O	2.11	0.49
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.94	0.49
2:B:190:TYR:CD1	8:J:62:ARG:HG2	2.48	0.49
2:B:204:ILE:O	2:B:205:ILE:HD13	2.12	0.49
1:A:369:SER:O	1:A:372:LYS:HB2	2.12	0.49
2:B:797:TYR:CE1	2:B:854:LEU:CD2	2.95	0.49
2:B:1000:PRO:O	2:B:1008:PRO:HD3	2.13	0.49
2:B:1152:MET:HE1	2:B:1195:HIS:HB3	1.94	0.49
1:A:332:LYS:C	1:A:334:GLY:H	2.20	0.49
1:A:780:VAL:HG23	1:A:789:LYS:HE2	1.94	0.49
2:B:734:HIS:O	2:B:735:ALA:CB	2.60	0.49
2:B:780:VAL:HG21	8:J:56:LEU:HD13	1.94	0.49
2:B:823:ALA:HA	8:J:48:ARG:HH12	1.77	0.49
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.48	0.49
7:I:7:CYS:SG	7:I:8:ARG:N	2.86	0.49
1:A:639:PRO:HG2	1:A:640:GLN:H	1.78	0.49
1:A:912:LEU:HD21	1:A:1033:GLN:HG3	1.94	0.49
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.41	0.49
2:B:57:TYR:CD1	2:B:57:TYR:N	2.81	0.49
2:B:380:TYR:CE1	2:B:384:ARG:HD3	2.48	0.49
2:B:482:VAL:C	2:B:483:LEU:O	2.56	0.49
2:B:805:THR:CG2	2:B:815:ARG:HH21	2.26	0.49
2:B:816:GLU:O	8:J:56:LEU:HD21	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:60:ALA:O	6:H:61:SER:HB3	2.12	0.49
10:L:30:ILE:HD12	10:L:57:LEU:HB2	1.95	0.49
1:A:129:LYS:O	1:A:130:ASP:HB2	2.12	0.48
1:A:265:LYS:C	1:A:267:ALA:N	2.68	0.48
1:A:315:LEU:HD12	1:A:319:GLY:HA2	1.95	0.48
1:A:538:ASP:HB2	6:H:20:TYR:HD2	1.78	0.48
2:B:34:ILE:CG1	2:B:542:MET:CE	2.90	0.48
2:B:999:MET:HE3	2:B:999:MET:CA	2.43	0.48
12:T:26:DA:C2	12:T:27:DT:C6	3.01	0.48
1:A:512:VAL:HG13	1:A:512:VAL:O	2.12	0.48
1:A:667:GLY:HA2	1:A:670:ILE:HG13	1.95	0.48
1:A:751:SER:OG	2:B:1015:HIS:HE1	1.96	0.48
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.38	0.48
1:A:1209:MET:HE3	1:A:1228:TRP:HB2	1.95	0.48
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.48	0.48
6:H:62:SER:OG	6:H:63:LEU:N	2.44	0.48
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.29	0.48
12:T:20:DC:H2'	12:T:21:DT:O4'	2.13	0.48
1:A:19:PHE:O	1:A:1416:ALA:HA	2.14	0.48
1:A:1341:ILE:HD13	1:A:1379:GLY:O	2.13	0.48
2:B:986:GLN:HG3	2:B:1025:HIS:CD2	2.49	0.48
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.49	0.48
1:A:503:GLN:O	1:A:509:LEU:CD1	2.60	0.48
1:A:1193:LEU:N	1:A:1260:LEU:HD21	2.29	0.48
2:B:459:TYR:C	2:B:459:TYR:HD2	2.19	0.48
2:B:516:ASN:HD22	2:B:516:ASN:N	2.10	0.48
2:B:708:GLU:C	2:B:710:LEU:N	2.71	0.48
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.92	0.48
2:B:808:ALA:C	2:B:810:GLU:N	2.72	0.48
3:C:54:ASN:OD1	3:C:63:ILE:HD12	2.14	0.48
1:A:84:ILE:HG13	1:A:270:LEU:HD13	1.95	0.48
1:A:637:LYS:HD2	1:A:641:VAL:HG11	1.96	0.48
1:A:668:ASP:CG	1:A:742:ASN:HD22	2.22	0.48
2:B:1074:ASN:ND2	2:B:1077:THR:H	2.11	0.48
4:E:180:ARG:NH2	4:E:192:ARG:HB2	2.28	0.48
4:E:187:TYR:CD2	4:E:187:TYR:O	2.67	0.48
4:E:205:SER:O	4:E:206:GLY:C	2.56	0.48
6:H:116:TYR:HB2	6:H:123:MET:HB3	1.96	0.48
8:J:64:ASN:HB3	8:J:65:PRO:HD3	1.96	0.48
9:K:70:ARG:O	9:K:70:ARG:HG3	2.12	0.48
1:A:540:PHE:CE1	6:H:43:ASN:ND2	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:826:ALA:O	2:B:1011:ILE:HA	2.14	0.48
2:B:834:ASN:HB3	2:B:839:MET:HA	1.95	0.48
4:E:161:LYS:HD2	4:E:195:VAL:CG2	2.44	0.48
6:H:40:LEU:HD13	6:H:123:MET:HE3	1.96	0.48
1:A:253:ASN:ND2	1:A:254:GLU:H	2.11	0.48
1:A:337:ARG:NH2	12:T:17:DC:OP1	2.46	0.48
1:A:535:THR:HG21	1:A:617:VAL:N	2.19	0.48
1:A:785:PRO:HG3	2:B:698:GLU:HG2	1.95	0.48
1:A:793:SER:CB	1:A:794:PRO:HD2	2.43	0.48
2:B:202:TYR:CD2	2:B:202:TYR:N	2.82	0.48
2:B:458:LYS:O	2:B:462:ALA:N	2.41	0.48
10:L:28:LYS:HE2	10:L:39:SER:OG	2.14	0.48
2:B:100:PRO:HD3	2:B:126:SER:HB3	1.95	0.48
2:B:115:GLN:O	2:B:119:LEU:HD12	2.14	0.48
2:B:542:MET:HG3	2:B:747:MET:HE3	1.96	0.48
2:B:827:ILE:HA	2:B:1012:ILE:O	2.14	0.48
3:C:251:LEU:HG	9:K:98:LEU:HD11	1.95	0.48
6:H:30:SER:HB2	6:H:36:CYS:SG	2.54	0.48
12:T:23:DT:C2	12:T:24:DC:C5	3.02	0.48
1:A:225:ASN:O	1:A:227:VAL:N	2.47	0.48
1:A:232:GLU:HG2	1:A:233:TRP:CD1	2.48	0.48
1:A:858:ASN:O	1:A:860:LEU:N	2.47	0.48
2:B:698:GLU:HA	2:B:701:ILE:HD12	1.96	0.48
2:B:879:ARG:HB2	2:B:880:THR:CB	2.44	0.48
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.46	0.48
2:B:992:ILE:CD1	9:K:67:PHE:HE2	2.27	0.48
3:C:69:LEU:HD23	8:J:6:ARG:HB2	1.96	0.48
3:C:98:VAL:CG1	3:C:99:LEU:H	2.26	0.48
1:A:106:VAL:HG11	1:A:214:ILE:HD12	1.96	0.47
1:A:757:ASN:HA	2:B:1021:MET:HE1	1.96	0.47
2:B:174:LEU:HD12	2:B:174:LEU:HA	1.59	0.47
2:B:236:HIS:HD2	2:B:389:ALA:HB2	1.77	0.47
2:B:551:PRO:O	2:B:554:ILE:HB	2.14	0.47
2:B:732:SER:HB3	2:B:734:HIS:HD2	1.79	0.47
7:I:10:CYS:HB2	7:I:31:THR:HG1	1.74	0.47
7:I:59:VAL:HG12	7:I:60:GLN:N	2.29	0.47
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.49	0.47
1:A:540:PHE:CZ	6:H:121:LEU:HD21	2.48	0.47
1:A:1192:LEU:HD11	1:A:1239:ARG:HH11	1.78	0.47
1:A:1263:ILE:HG23	1:A:1264:GLU:N	2.28	0.47
1:A:1364:ASN:HD21	1:A:1366:ARG:HG2	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:84:ARG:HG3	3:C:85:ASP:N	2.29	0.47
6:H:82:PRO:C	6:H:84:ALA:N	2.71	0.47
1:A:786:HIS:CE1	2:B:705:MET:SD	3.07	0.47
2:B:193:LYS:HD3	2:B:787:VAL:HG11	1.95	0.47
2:B:240:ILE:C	2:B:240:ILE:HD13	2.39	0.47
2:B:541:LEU:HB3	2:B:747:MET:HE1	1.95	0.47
2:B:1032:SER:O	2:B:1033:LYS:C	2.57	0.47
3:C:14:SER:OG	3:C:17:ASN:HB2	2.14	0.47
9:K:74:ARG:C	9:K:75:ILE:HG13	2.38	0.47
1:A:264:PHE:HE1	1:A:317:LYS:CB	2.11	0.47
1:A:363:GLN:HG3	1:A:459:ARG:NH1	2.30	0.47
1:A:575:LYS:CB	1:A:612:ILE:HD11	2.42	0.47
2:B:248:SER:H	2:B:418:LYS:NZ	2.03	0.47
2:B:701:ILE:HB	2:B:739:THR:OG1	2.14	0.47
2:B:1084:GLN:NE2	3:C:191:TYR:HA	2.28	0.47
3:C:178:PHE:C	3:C:178:PHE:HD2	2.23	0.47
4:E:46:TYR:CD2	4:E:58:MET:HG3	2.49	0.47
4:E:77:SER:HB3	4:E:105:PHE:HA	1.97	0.47
4:E:166:LYS:O	4:E:169:ARG:N	2.45	0.47
1:A:26:GLU:O	1:A:30:ILE:HB	2.15	0.47
1:A:344:ARG:HB3	2:B:1118:PRO:HG2	1.97	0.47
1:A:452:LYS:HE2	1:A:510:GLN:HE22	1.79	0.47
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.97	0.47
1:A:1031:VAL:HG22	1:A:1031:VAL:O	2.14	0.47
2:B:97:VAL:HB	2:B:178:ASN:HD21	1.79	0.47
2:B:115:GLN:OE1	2:B:115:GLN:HA	2.15	0.47
2:B:679:TYR:HE1	2:B:687:GLU:OE2	1.98	0.47
1:A:344:ARG:CZ	2:B:1129:ARG:HB2	2.44	0.47
1:A:840:ARG:O	1:A:841:LEU:C	2.56	0.47
2:B:316:PRO:HA	2:B:319:GLU:HG3	1.97	0.47
2:B:472:ALA:O	2:B:474:SER:HB3	2.15	0.47
2:B:542:MET:HG3	2:B:747:MET:HE2	1.96	0.47
6:H:113:ALA:HA	6:H:125:LEU:O	2.15	0.47
1:A:343:LYS:NZ	2:B:1197:PRO:HB3	2.30	0.47
1:A:350:ARG:HH21	12:T:21:DT:H2"	1.79	0.47
1:A:357:PRO:HB3	1:A:472:LEU:HD11	1.97	0.47
1:A:451:HIS:C	1:A:453:MET:H	2.23	0.47
1:A:711:ARG:NH1	7:I:91:ARG:HH12	2.13	0.47
1:A:726:ARG:HH11	1:A:766:GLY:HA3	1.79	0.47
1:A:775:ILE:CG1	1:A:798:GLY:HA3	2.42	0.47
1:A:1203:ASN:O	1:A:1204:ASP:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1338:VAL:O	4:E:183:PRO:HB3	2.14	0.47
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	1.96	0.47
2:B:174:LEU:HD22	2:B:204:ILE:CD1	2.44	0.47
2:B:360:PHE:O	2:B:361:LEU:C	2.57	0.47
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.44	0.47
2:B:628:THR:HG23	2:B:628:THR:O	2.14	0.47
2:B:636:PRO:CB	2:B:637:LEU:CA	2.65	0.47
2:B:726:ALA:CB	2:B:1051:THR:HG21	2.45	0.47
2:B:955:THR:HG23	10:L:54:ARG:O	2.15	0.47
2:B:975:GLN:N	2:B:978:ASP:OD2	2.40	0.47
4:E:181:ALA:HA	4:E:186:LEU:HD21	1.97	0.47
6:H:112:ILE:N	6:H:127:GLY:O	2.31	0.47
9:K:19:LEU:HD22	9:K:33:ILE:HG22	1.95	0.47
1:A:998:LEU:HD12	1:A:1001:ARG:HG3	1.97	0.47
2:B:475:SER:O	2:B:476:ARG:C	2.58	0.47
2:B:763:GLN:HB2	2:B:1021:MET:HB2	1.97	0.47
2:B:952:VAL:CG1	2:B:953:LEU:N	2.78	0.47
3:C:189:THR:HG22	3:C:190:ASP:N	2.30	0.47
3:C:244:VAL:O	3:C:248:ILE:HG13	2.15	0.47
7:I:111:THR:HG22	7:I:112:SER:N	2.29	0.47
1:A:645:LEU:O	1:A:646:PHE:C	2.57	0.47
1:A:774:ARG:NH2	1:A:797:LYS:HD3	2.30	0.47
1:A:1155:ASP:OD2	1:A:1162:VAL:HG23	2.14	0.47
2:B:210:LYS:HA	2:B:481:GLN:O	2.15	0.47
2:B:1110:PRO:O	2:B:1119:VAL:HG12	2.14	0.47
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.97	0.47
6:H:109:LYS:HB2	6:H:111:LEU:N	2.29	0.47
6:H:128:ASN:O	6:H:131:ASN:ND2	2.47	0.47
1:A:457:ALA:HB3	1:A:506:ALA:CA	2.43	0.47
1:A:830:LYS:HD3	1:A:1080:THR:HA	1.97	0.47
1:A:840:ARG:HG2	1:A:1402:PHE:HZ	1.80	0.47
1:A:913:LEU:HD11	1:A:981:LEU:O	2.14	0.47
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.80	0.47
2:B:468:GLU:HG3	2:B:469:GLN:N	2.29	0.47
2:B:658:ILE:HD12	2:B:661:LEU:HD12	1.97	0.47
2:B:789:MET:HE1	2:B:967:ARG:HB3	1.97	0.47
2:B:992:ILE:HD11	9:K:67:PHE:CE2	2.49	0.47
3:C:93:ASP:O	3:C:127:ARG:NH2	2.47	0.47
7:I:71:SER:H	7:I:83:ASN:ND2	2.13	0.47
11:R:7:A:H2'	11:R:8:G:H5'	1.97	0.47
1:A:830:LYS:HD3	1:A:1079:MET:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:ASN:ND2	1:A:906:HIS:HB2	2.30	0.46
2:B:956:THR:HG23	2:B:961:LEU:H	1.80	0.46
2:B:1077:THR:HG22	2:B:1079:LYS:HB2	1.97	0.46
3:C:30:ALA:O	3:C:230:MET:HE1	2.15	0.46
1:A:91:PHE:HA	1:A:235:ILE:HG22	1.96	0.46
1:A:106:VAL:HG11	1:A:214:ILE:CD1	2.44	0.46
1:A:106:VAL:HG12	1:A:107:CYS:N	2.30	0.46
1:A:253:ASN:CG	1:A:254:GLU:N	2.70	0.46
1:A:618:GLU:O	1:A:622:VAL:HG12	2.15	0.46
1:A:845:LEU:O	1:A:848:ILE:HD13	2.15	0.46
1:A:933:TYR:CD2	1:A:933:TYR:O	2.68	0.46
2:B:481:GLN:CD	2:B:494:HIS:HE2	2.23	0.46
2:B:1135:ARG:NE	2:B:1139:ILE:HD11	2.30	0.46
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.50	0.46
5:F:75:PRO:O	5:F:79:ARG:HD2	2.15	0.46
6:H:109:LYS:HB3	6:H:110:ASP:CA	2.45	0.46
11:R:9:G:H5'	11:R:10:A:OP2	2.15	0.46
1:A:92:HIS:O	1:A:94:GLY:N	2.49	0.46
1:A:445:ASN:OD1	1:A:455:MET:HE2	2.16	0.46
1:A:582:ILE:HD12	1:A:629:LEU:HD11	1.97	0.46
1:A:630:ILE:CD1	1:A:630:ILE:N	2.71	0.46
1:A:1394:THR:HG22	1:A:1395:GLY:H	1.79	0.46
2:B:113:TYR:O	2:B:114:PRO:C	2.56	0.46
2:B:459:TYR:O	2:B:459:TYR:HD2	1.98	0.46
2:B:798:TYR:HE2	3:C:66:ARG:HH21	1.62	0.46
3:C:148:ARG:HD2	3:C:149:LYS:H	1.81	0.46
1:A:49:LYS:O	1:A:50:ILE:HB	2.14	0.46
1:A:315:LEU:HB3	1:A:317:LYS:N	2.31	0.46
1:A:525:GLN:O	1:A:528:LEU:N	2.48	0.46
2:B:31:TRP:CD1	2:B:807:ARG:HH11	2.33	0.46
2:B:199:MET:HE2	2:B:492:LEU:HD23	1.98	0.46
2:B:287:ARG:NH2	2:B:294:ASP:OD2	2.49	0.46
2:B:307:ASP:O	2:B:310:MET:HB3	2.15	0.46
2:B:732:SER:HB3	2:B:734:HIS:CD2	2.51	0.46
2:B:827:ILE:CD1	2:B:1086:PHE:HD2	2.28	0.46
2:B:976:ILE:HD11	2:B:992:ILE:HD12	1.97	0.46
2:B:1146:PHE:CD2	2:B:1146:PHE:C	2.93	0.46
4:E:61:GLN:HE21	4:E:105:PHE:HZ	1.63	0.46
1:A:344:ARG:NH1	2:B:1129:ARG:HB2	2.30	0.46
1:A:417:TYR:O	1:A:418:SER:HB3	2.15	0.46
1:A:827:THR:HG21	11:R:11:G:CI'	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:784:ASN:OD1	2:B:788:ARG:HG3	2.15	0.46
1:A:108:MET:C	1:A:110:CYS:H	2.23	0.46
1:A:440:ASP:O	1:A:460:VAL:HG23	2.15	0.46
1:A:626:ASN:O	1:A:631:HIS:CD2	2.69	0.46
1:A:767:GLN:OE1	1:A:774:ARG:HD2	2.15	0.46
1:A:1019:CYS:O	1:A:1023:ARG:HG3	2.16	0.46
2:B:708:GLU:CG	2:B:709:ASP:H	2.27	0.46
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.14	0.46
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.51	0.46
7:I:10:CYS:CB	7:I:31:THR:HG1	2.29	0.46
1:A:1042:PHE:C	1:A:1042:PHE:CD2	2.94	0.46
2:B:236:HIS:NE2	2:B:389:ALA:HA	2.31	0.46
3:C:248:ILE:HG13	3:C:248:ILE:H	1.60	0.46
1:A:982:THR:C	1:A:984:LYS:H	2.24	0.46
1:A:1427:ASN:CB	1:A:1434:ALA:HB2	2.44	0.46
2:B:843:GLN:HB2	2:B:993:THR:OG1	2.16	0.46
3:C:29:MET:HB3	9:K:45:LEU:HD11	1.98	0.46
1:A:339:ASN:O	1:A:343:LYS:HG2	2.16	0.46
1:A:533:LYS:HE3	1:A:745:GLN:HE22	1.81	0.46
1:A:834:THR:O	1:A:834:THR:HG22	2.15	0.46
1:A:857:ARG:HA	1:A:864:ILE:HD12	1.98	0.46
2:B:232:SER:OG	2:B:234:ILE:O	2.34	0.46
2:B:642:ASP:O	2:B:644:GLU:N	2.49	0.46
3:C:88:CYS:SG	3:C:92:CYS:HB3	2.56	0.46
3:C:204:SER:C	3:C:206:ASN:N	2.72	0.46
7:I:69:PRO:HG2	7:I:85:PHE:CE1	2.50	0.46
1:A:577:ILE:O	1:A:580:VAL:N	2.39	0.46
1:A:645:LEU:CG	1:A:649:ILE:HD11	2.42	0.46
1:A:751:SER:CB	2:B:1015:HIS:CE1	3.00	0.46
1:A:1042:PHE:O	1:A:1045:VAL:N	2.49	0.46
2:B:593:PRO:HA	2:B:596:LEU:HB3	1.98	0.46
2:B:704:ALA:HB1	2:B:710:LEU:HD13	1.74	0.46
4:E:168:TYR:C	4:E:169:ARG:HG2	2.41	0.46
9:K:24:ASP:OD2	9:K:74:ARG:HD2	2.15	0.46
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.98	0.45
2:B:522:VAL:HG13	2:B:537:LYS:HB2	1.97	0.45
3:C:244:VAL:HG21	9:K:105:PHE:CZ	2.52	0.45
5:F:89:GLU:O	5:F:93:ILE:HG12	2.16	0.45
7:I:63:GLY:HA3	7:I:104:LEU:CD1	2.40	0.45
1:A:472:LEU:HD22	2:B:835:GLN:CB	2.46	0.45
1:A:527:THR:HG23	1:A:653:VAL:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ASP:OD1	1:A:559:VAL:HG22	2.17	0.45
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.97	0.45
1:A:830:LYS:HD3	1:A:1080:THR:OG1	2.17	0.45
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.97	0.45
2:B:1119:VAL:O	2:B:1126:GLY:CA	2.65	0.45
2:B:1138:MET:HB3	2:B:1147:LEU:HD12	1.98	0.45
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.99	0.45
1:A:596:THR:C	1:A:598:LEU:N	2.74	0.45
2:B:230:ALA:C	2:B:232:SER:H	2.23	0.45
2:B:287:ARG:HB3	2:B:330:ALA:HB2	1.99	0.45
3:C:31:ASN:O	3:C:34:ARG:N	2.49	0.45
11:R:7:A:C2'	11:R:8:G:H5'	2.46	0.45
1:A:531:ILE:O	1:A:535:THR:HB	2.16	0.45
2:B:345:LYS:N	2:B:347:LYS:HE3	2.32	0.45
2:B:546:SER:N	2:B:634:TYR:HE2	2.14	0.45
2:B:977:GLY:HA3	2:B:1099:VAL:HG11	1.97	0.45
3:C:54:ASN:C	3:C:54:ASN:ND2	2.69	0.45
3:C:101:LEU:HD21	3:C:113:VAL:HG11	1.98	0.45
4:E:198:ILE:HD11	4:E:212:ARG:HG3	1.93	0.45
9:K:6:ARG:HH11	9:K:6:ARG:HB3	1.81	0.45
9:K:7:PHE:C	9:K:9:LEU:H	2.24	0.45
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.97	0.45
1:A:47:ARG:HB2	1:A:47:ARG:HH11	1.81	0.45
1:A:224:PHE:HZ	1:A:234:MET:HE3	1.79	0.45
1:A:629:LEU:O	1:A:633:VAL:HG23	2.17	0.45
1:A:767:GLN:NE2	1:A:797:LYS:O	2.49	0.45
1:A:1434:ALA:O	1:A:1436:ILE:N	2.50	0.45
2:B:210:LYS:HE3	2:B:462:ALA:HA	1.97	0.45
2:B:273:LEU:HD23	2:B:274:PRO:HD2	1.98	0.45
2:B:426:LYS:HD2	2:B:430:ARG:HH22	1.82	0.45
2:B:494:HIS:HA	2:B:497:ARG:CZ	2.46	0.45
2:B:778:MET:HG2	2:B:794:ASN:HB3	1.97	0.45
2:B:1097:HIS:HB3	2:B:1102:LYS:NZ	2.31	0.45
3:C:167:HIS:HD2	3:C:169:LYS:N	2.07	0.45
4:E:187:TYR:HD2	4:E:188:LEU:HG	1.80	0.45
5:F:90:ARG:HD3	5:F:155:LEU:HD11	1.97	0.45
6:H:41:ASP:O	6:H:121:LEU:HD12	2.17	0.45
1:A:532:ARG:O	1:A:533:LYS:C	2.59	0.45
1:A:814:PHE:O	1:A:818:MET:HG3	2.16	0.45
1:A:1004:ASN:HD22	4:E:167:ARG:HH11	1.65	0.45
2:B:1115:THR:O	2:B:1116:ARG:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:LYS:H	3:C:15:LYS:HD2	1.80	0.45
3:C:43:THR:HG22	3:C:44:LEU:N	2.32	0.45
6:H:98:TYR:C	6:H:118:PHE:HD2	2.25	0.45
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.97	0.45
1:A:635:ARG:HA	1:A:635:ARG:NH1	2.29	0.45
1:A:660:ASN:HA	2:B:1082:MET:HB2	1.99	0.45
1:A:853:ASP:C	1:A:855:THR:H	2.24	0.45
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.98	0.45
1:A:1030:ARG:C	1:A:1032:LEU:H	2.23	0.45
2:B:273:LEU:HD21	2:B:360:PHE:CD1	2.52	0.45
2:B:321:GLY:O	2:B:323:VAL:N	2.50	0.45
2:B:726:ALA:HB1	2:B:1051:THR:CG2	2.46	0.45
2:B:1162:ILE:HD11	2:B:1216:LEU:HD23	1.99	0.45
3:C:258:ILE:HD11	9:K:19:LEU:HD11	1.99	0.45
12:T:17:DC:O2	12:T:17:DC:H2'	2.16	0.45
1:A:545:GLN:HB3	1:A:549:MET:HE3	1.99	0.45
1:A:760:GLN:NE2	1:A:765:VAL:O	2.49	0.45
1:A:1120:LEU:HB3	1:A:1124:HIS:O	2.17	0.45
2:B:375:ALA:O	2:B:376:PHE:C	2.60	0.45
2:B:850:LEU:O	2:B:974:PRO:HG2	2.16	0.45
3:C:51:VAL:O	10:L:64:LEU:HD22	2.17	0.45
3:C:258:ILE:O	3:C:258:ILE:HD13	2.17	0.45
4:E:12:LEU:CD2	4:E:53:PRO:HB3	2.46	0.45
7:I:68:LEU:HA	7:I:69:PRO:HD3	1.70	0.45
8:J:7:CYS:HA	8:J:49:MET:HG2	1.98	0.45
1:A:1274:ARG:HB3	1:A:1274:ARG:NH1	2.32	0.45
2:B:487:THR:HG21	2:B:819:ALA:CB	2.47	0.45
2:B:1065:GLN:HG2	3:C:201:TRP:CZ3	2.52	0.45
3:C:177:GLU:OE2	8:J:42:LYS:NZ	2.45	0.45
1:A:356:ASP:OD2	1:A:359:LEU:HG	2.16	0.45
1:A:380:VAL:HG13	1:A:385:ILE:HG23	1.99	0.45
1:A:467:THR:HG22	2:B:1099:VAL:HG11	1.99	0.45
1:A:1032:LEU:O	1:A:1036:ARG:HG2	2.18	0.45
2:B:857:ARG:HD2	2:B:945:GLU:OE1	2.17	0.45
2:B:1138:MET:HA	2:B:1138:MET:CE	2.40	0.45
4:E:79:TRP:CD1	4:E:100:ILE:HD11	2.51	0.45
4:E:196:VAL:HG12	4:E:197:LYS:N	2.32	0.45
8:J:36:LEU:O	8:J:41:LEU:HB2	2.16	0.45
10:L:38:LEU:HD21	10:L:48:CYS:HA	1.99	0.45
1:A:494:SER:HB2	2:B:1149:GLU:OE2	2.17	0.44
1:A:512:VAL:HA	1:A:519:PRO:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ILE:HG22	1:A:528:LEU:HB2	1.99	0.44
1:A:780:VAL:O	1:A:789:LYS:HG2	2.17	0.44
2:B:33:VAL:HG23	2:B:658:ILE:HD11	1.99	0.44
2:B:801:LYS:O	8:J:52:THR:HG23	2.16	0.44
2:B:1152:MET:CE	2:B:1195:HIS:HB3	2.47	0.44
2:B:1160:VAL:HG11	2:B:1169:MET:SD	2.57	0.44
3:C:29:MET:HG3	3:C:30:ALA:N	2.31	0.44
4:E:14:ARG:NH1	4:E:142:VAL:HG22	2.20	0.44
1:A:1340:GLY:O	1:A:1341:ILE:C	2.60	0.44
2:B:569:TYR:HE1	2:B:574:SER:HB2	1.82	0.44
2:B:597:MET:O	2:B:600:LEU:N	2.50	0.44
5:F:89:GLU:OE2	5:F:136:ARG:NE	2.50	0.44
1:A:562:THR:HA	1:A:563:PRO:HD3	1.86	0.44
1:A:628:GLY:O	1:A:632:VAL:HG23	2.17	0.44
1:A:1116:LEU:HB2	1:A:1308:THR:CG2	2.48	0.44
2:B:169:ARG:HH11	2:B:169:ARG:HG2	1.73	0.44
2:B:288:ALA:HB1	2:B:331:LEU:HD13	1.98	0.44
2:B:622:LYS:HE3	7:I:57:GLY:HA2	1.99	0.44
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.16	0.44
2:B:997:GLU:HG2	3:C:39:ALA:CB	2.44	0.44
2:B:1177:HIS:O	2:B:1179:GLN:N	2.50	0.44
3:C:115:SER:HB3	3:C:142:VAL:HB	1.99	0.44
5:F:88:TYR:O	5:F:89:GLU:C	2.61	0.44
11:R:4:G:H2'	11:R:5:A:C8	2.53	0.44
1:A:27:VAL:HG12	1:A:83:HIS:HB2	1.99	0.44
1:A:79:GLY:O	1:A:243:PRO:HG3	2.17	0.44
1:A:395:GLY:C	1:A:397:ASN:H	2.25	0.44
1:A:559:VAL:O	1:A:560:ILE:C	2.60	0.44
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.99	0.44
2:B:261:ARG:HB2	2:B:264:SER:HB2	1.98	0.44
2:B:730:ARG:HB2	2:B:730:ARG:NH1	2.32	0.44
2:B:1022:THR:HG23	2:B:1022:THR:O	2.18	0.44
4:E:147:HIS:HD2	4:E:149:LEU:H	1.66	0.44
1:A:246:VAL:O	1:A:246:VAL:HG12	2.17	0.44
1:A:362:ASP:OD2	1:A:362:ASP:N	2.35	0.44
1:A:461:LYS:HG3	1:A:461:LYS:O	2.16	0.44
2:B:301:ILE:HG22	2:B:302:CYS:N	2.31	0.44
3:C:142:VAL:H	8:J:16:ASP:CB	2.27	0.44
4:E:75:MET:CG	4:E:76:GLY:N	2.79	0.44
6:H:40:LEU:HD21	6:H:142:LEU:HD21	1.99	0.44
7:I:75:CYS:HA	7:I:76:PRO:HD2	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:99:LEU:O	7:I:111:THR:HG23	2.18	0.44
8:J:1:MET:HG3	8:J:60:PHE:CE2	2.53	0.44
11:R:10:A:H5'	11:R:11:G:OP2	2.17	0.44
1:A:67:CYS:HB3	1:A:80:HIS:CE1	2.53	0.44
1:A:773:LYS:C	1:A:774:ARG:O	2.61	0.44
1:A:888:GLY:O	1:A:889:SER:O	2.35	0.44
1:A:1100:ARG:O	1:A:1103:GLU:N	2.51	0.44
1:A:1154:TYR:HB2	1:A:1191:TRP:CZ3	2.53	0.44
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.17	0.44
2:B:94:LYS:HA	2:B:94:LYS:HD2	1.84	0.44
2:B:273:LEU:HD21	2:B:360:PHE:HD1	1.81	0.44
2:B:654:ARG:HD3	2:B:654:ARG:HA	1.83	0.44
2:B:957:ASN:H	2:B:961:LEU:HB2	1.81	0.44
2:B:976:ILE:HD12	2:B:993:THR:HG22	1.98	0.44
3:C:45:ALA:O	3:C:46:ILE:C	2.60	0.44
3:C:148:ARG:HB2	3:C:151:GLN:CD	2.43	0.44
5:F:81:THR:HG22	5:F:136:ARG:HD3	1.99	0.44
11:R:1:A:C5	11:R:2:U:C5	3.05	0.44
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.48	0.44
2:B:796:LEU:HD23	2:B:799:PRO:HA	2.00	0.44
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.99	0.44
1:A:33:ALA:O	1:A:83:HIS:CD2	2.70	0.44
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.32	0.44
1:A:1134:ILE:O	1:A:1135:ARG:C	2.60	0.44
1:A:1212:VAL:HA	1:A:1273:LEU:HD21	1.98	0.44
1:A:1397:LEU:O	1:A:1400:CYS:HB3	2.17	0.44
1:A:1398:MET:O	1:A:1401:SER:N	2.45	0.44
2:B:1204:PHE:O	2:B:1208:MET:HB2	2.17	0.44
3:C:44:LEU:HD12	3:C:160:LYS:C	2.43	0.44
4:E:75:MET:HG3	4:E:76:GLY:N	2.33	0.44
4:E:113:GLN:HA	4:E:137:GLU:CG	2.47	0.44
8:J:5:VAL:HG12	8:J:6:ARG:HG3	2.00	0.44
10:L:46:VAL:HG22	10:L:47:ARG:N	2.25	0.44
1:A:672:ASP:HB2	1:A:736:ASN:HD21	1.82	0.44
1:A:805:LEU:C	1:A:805:LEU:HD12	2.43	0.44
1:A:908:LEU:HD22	1:A:1032:LEU:HD12	2.00	0.44
1:A:919:ILE:O	1:A:920:LEU:C	2.60	0.44
1:A:928:LEU:HA	1:A:931:GLU:HB3	1.99	0.44
2:B:520:GLY:O	2:B:521:LEU:HD23	2.17	0.44
2:B:997:GLU:CG	3:C:39:ALA:HB2	2.44	0.44
3:C:131:HIS:HA	3:C:132:PRO:HD2	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:14:LEU:HD22	7:I:29:CYS:HB2	1.99	0.44
1:A:577:ILE:O	1:A:578:LEU:C	2.61	0.43
1:A:633:VAL:HG11	1:A:645:LEU:HD22	2.00	0.43
1:A:954:TRP:HA	1:A:955:PRO:HD2	1.82	0.43
1:A:1101:LEU:HG	1:A:1105:LEU:HD11	2.00	0.43
1:A:1397:LEU:HB2	1:A:1426:GLU:HG2	2.00	0.43
2:B:232:SER:HA	2:B:233:PRO:HD2	1.88	0.43
2:B:473:MET:CA	2:B:474:SER:HB3	2.46	0.43
2:B:983:ARG:HD2	2:B:1091:TYR:CB	2.35	0.43
2:B:1059:LEU:HA	2:B:1062:HIS:HB2	1.99	0.43
1:A:577:ILE:C	1:A:579:SER:N	2.76	0.43
1:A:649:ILE:O	1:A:653:VAL:HG22	2.18	0.43
1:A:744:LYS:CE	1:A:748:MET:HE3	2.47	0.43
1:A:900:ASP:O	1:A:907:THR:HA	2.18	0.43
1:A:1152:ILE:O	1:A:1152:ILE:HG22	2.18	0.43
7:I:78:CYS:O	7:I:79:HIS:HB2	2.19	0.43
1:A:265:LYS:O	1:A:268:ASP:N	2.51	0.43
1:A:272:ALA:HA	1:A:275:SER:HB3	2.00	0.43
1:A:351:THR:HG23	2:B:1103:ILE:HD13	1.99	0.43
1:A:472:LEU:HD13	2:B:835:GLN:HE22	1.81	0.43
1:A:741:ASN:O	1:A:744:LYS:HB2	2.18	0.43
1:A:1195:LEU:O	1:A:1237:ILE:HA	2.19	0.43
1:A:1404:GLU:HB3	1:A:1407:GLU:CG	2.49	0.43
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.17	0.43
1:A:67:CYS:HB3	1:A:80:HIS:HE1	1.83	0.43
1:A:81:PHE:CE1	2:B:1208:MET:HG2	2.54	0.43
1:A:613:ILE:O	6:H:117:SER:OG	2.31	0.43
2:B:361:LEU:HD11	2:B:381:MET:HE3	1.99	0.43
2:B:376:PHE:HB3	2:B:586:TRP:CZ3	2.53	0.43
2:B:386:LEU:C	2:B:388:CYS:N	2.75	0.43
2:B:913:GLY:HA2	2:B:938:SER:CB	2.48	0.43
5:F:75:PRO:C	5:F:77:ASP:H	2.26	0.43
1:A:305:ASP:OD1	1:A:306:ASN:N	2.51	0.43
1:A:403:LYS:O	1:A:404:TYR:CB	2.57	0.43
1:A:650:GLN:O	1:A:651:LYS:C	2.61	0.43
1:A:660:ASN:O	2:B:1081:LEU:HD22	2.18	0.43
1:A:1323:ASP:HA	1:A:1324:PRO:HD3	1.88	0.43
1:A:1445:ILE:H	1:A:1445:ILE:HG13	1.71	0.43
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.99	0.43
2:B:126:SER:OG	2:B:172:ILE:HD11	2.18	0.43
2:B:565:PRO:HB2	2:B:567:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:SER:HB3	1:A:223:GLY:HA2	2.00	0.43
1:A:369:SER:HB3	9:K:2:ASN:ND2	2.30	0.43
1:A:456:MET:HG3	1:A:478:TYR:OH	2.18	0.43
1:A:932:GLU:O	1:A:934:LYS:N	2.51	0.43
1:A:1038:THR:O	1:A:1039:LYS:C	2.62	0.43
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	2.00	0.43
1:A:1341:ILE:CD1	1:A:1380:GLY:HA2	2.48	0.43
2:B:515:HIS:H	2:B:518:HIS:CD2	2.23	0.43
2:B:1081:LEU:HD23	2:B:1081:LEU:HA	1.89	0.43
2:B:1098:MET:O	2:B:1099:VAL:C	2.62	0.43
3:C:262:LEU:HD21	9:K:87:LEU:HD23	2.00	0.43
1:A:401:GLY:H	1:A:435:HIS:HD2	1.66	0.43
1:A:894:GLU:C	1:A:896:ARG:H	2.24	0.43
2:B:57:TYR:N	2:B:57:TYR:HD1	2.15	0.43
2:B:102:VAL:HG22	2:B:112:LEU:HB2	2.00	0.43
2:B:621:GLU:HG3	2:B:623:GLU:HG3	2.00	0.43
2:B:788:ARG:HH11	2:B:788:ARG:CG	2.32	0.43
7:I:111:THR:HG22	7:I:112:SER:H	1.82	0.43
8:J:7:CYS:HB2	8:J:49:MET:HG2	2.01	0.43
11:R:7:A:N6	12:T:21:DT:H3	2.16	0.43
1:A:58:LEU:CD2	1:A:244:PRO:HD2	2.48	0.43
1:A:336:ILE:HD11	2:B:1203:LEU:HD13	2.01	0.43
1:A:447:GLN:HA	1:A:448:PRO:C	2.43	0.43
1:A:783:THR:O	2:B:516:ASN:OD1	2.36	0.43
1:A:810:PRO:O	1:A:811:GLN:C	2.61	0.43
1:A:1139:GLU:OE2	1:A:1282:VAL:HG12	2.18	0.43
2:B:707:PRO:CB	2:B:741:CYS:SG	3.00	0.43
6:H:137:GLN:HB2	6:H:138:GLU:H	1.69	0.43
8:J:64:ASN:HB3	8:J:65:PRO:CD	2.49	0.43
1:A:14:VAL:HG21	2:B:1216:LEU:HD12	2.00	0.43
1:A:58:LEU:C	1:A:58:LEU:CD2	2.91	0.43
1:A:265:LYS:HZ3	1:A:322:VAL:HG12	1.80	0.43
1:A:329:LEU:HD11	2:B:1203:LEU:HD12	2.01	0.43
1:A:590:ARG:HH21	1:A:621:THR:HA	1.84	0.43
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.49	0.43
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.84	0.43
2:B:199:MET:SD	2:B:200:GLY:N	2.92	0.43
2:B:235:SER:HA	2:B:261:ARG:HH21	1.83	0.43
2:B:240:ILE:HG23	2:B:240:ILE:O	2.18	0.43
2:B:562:GLY:O	2:B:563:MET:C	2.62	0.43
2:B:1132:GLU:H	2:B:1132:GLU:HG3	1.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLN:HB3	1:A:314:ALA:H	1.58	0.43
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.53	0.43
1:A:511:ILE:O	1:A:519:PRO:HA	2.19	0.43
1:A:800:VAL:HG11	1:A:808:LEU:HG	2.00	0.43
1:A:1209:MET:HG3	1:A:1236:LEU:HD22	2.01	0.43
2:B:212:LEU:HD21	2:B:466:TRP:CH2	2.53	0.43
2:B:635:ARG:O	2:B:636:PRO:C	2.62	0.43
2:B:797:TYR:OH	2:B:971:THR:OG1	2.31	0.43
5:F:101:ILE:HD13	5:F:120:ILE:HG22	2.00	0.43
6:H:12:VAL:HG22	6:H:53:ASP:O	2.19	0.43
7:I:61:ASP:O	7:I:62:ILE:C	2.62	0.43
8:J:53:HIS:CE1	8:J:55:ASP:HA	2.54	0.43
12:T:27:DT:H2'	12:T:27:DT:O2	2.19	0.43
1:A:269:ILE:HG23	1:A:299:HIS:CB	2.49	0.42
1:A:567:LYS:HE2	6:H:96:VAL:C	2.44	0.42
1:A:626:ASN:O	1:A:631:HIS:HD2	2.03	0.42
1:A:768:GLN:CG	1:A:816:HIS:HA	2.45	0.42
1:A:899:VAL:CG1	1:A:899:VAL:O	2.67	0.42
1:A:939:ASP:CG	1:A:1020:CYS:HB3	2.43	0.42
1:A:962:ARG:C	1:A:964:ILE:N	2.76	0.42
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.83	0.42
1:A:1191:TRP:CE3	1:A:1191:TRP:HA	2.53	0.42
2:B:23:ALA:HB1	2:B:24:PRO:CD	2.44	0.42
2:B:315:LYS:N	2:B:316:PRO:CD	2.81	0.42
2:B:515:HIS:HD2	2:B:517:THR:H	1.64	0.42
2:B:1131:GLY:O	2:B:1132:GLU:C	2.61	0.42
6:H:139:ASN:O	6:H:140:ALA:CB	2.65	0.42
1:A:457:ALA:HB3	1:A:506:ALA:N	2.34	0.42
1:A:552:TRP:CD1	1:A:655:PHE:CD1	3.07	0.42
1:A:737:LEU:HB3	1:A:744:LYS:HG3	2.01	0.42
1:A:928:LEU:O	1:A:931:GLU:HB3	2.19	0.42
1:A:1266:THR:O	1:A:1270:ASN:HB2	2.19	0.42
2:B:585:VAL:HG12	2:B:587:HIS:CD2	2.54	0.42
2:B:685:LEU:HD22	2:B:692:TYR:CE2	2.54	0.42
4:E:199:ILE:O	4:E:199:ILE:CG2	2.64	0.42
6:H:6:PHE:CG	6:H:7:ASP:N	2.86	0.42
6:H:93:TYR:CG	6:H:143:LEU:HB3	2.54	0.42
1:A:614:PHE:CD1	1:A:614:PHE:C	2.96	0.42
1:A:645:LEU:HG	1:A:649:ILE:CD1	2.43	0.42
1:A:818:MET:HE2	1:A:818:MET:HB3	1.85	0.42
1:A:848:ILE:HG21	1:A:1370:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.85	0.42
1:A:907:THR:HG22	1:A:908:LEU:H	1.85	0.42
1:A:1436:ILE:O	1:A:1438:THR:N	2.52	0.42
2:B:27:ALA:HB2	2:B:708:GLU:HG2	2.00	0.42
2:B:482:VAL:O	2:B:483:LEU:O	2.36	0.42
2:B:879:ARG:N	2:B:879:ARG:NE	2.67	0.42
2:B:1154:ALA:O	2:B:1155:SER:CB	2.66	0.42
4:E:83:CYS:SG	4:E:110:PHE:HE1	2.41	0.42
6:H:51:ALA:O	6:H:52:GLN:C	2.63	0.42
9:K:6:ARG:NH1	9:K:6:ARG:HB3	2.33	0.42
1:A:37:PHE:HB2	1:A:52:GLY:HA3	2.01	0.42
1:A:95:PHE:HB3	1:A:234:MET:HG2	2.01	0.42
1:A:388:LEU:HD13	1:A:391:LEU:HD12	2.02	0.42
1:A:683:ILE:HG21	1:A:801:GLU:HG2	2.01	0.42
1:A:709:THR:CG2	7:I:94:ASP:HA	2.46	0.42
1:A:824:LEU:O	11:R:11:G:N2	2.51	0.42
2:B:255:GLN:H	2:B:272:THR:HG22	1.84	0.42
2:B:372:SER:O	2:B:376:PHE:HD1	2.03	0.42
2:B:428:ILE:CD1	2:B:448:ILE:HD13	2.46	0.42
2:B:788:ARG:HG3	2:B:788:ARG:HH11	1.84	0.42
2:B:821:GLN:NE2	2:B:851:PHE:H	2.16	0.42
2:B:865:LYS:HB3	2:B:866:TYR:H	1.72	0.42
7:I:10:CYS:HB3	7:I:32:CYS:HB3	1.80	0.42
8:J:8:PHE:CD1	8:J:49:MET:HE1	2.54	0.42
8:J:16:ASP:OD2	8:J:17:LYS:HD2	2.20	0.42
1:A:88:LYS:HA	1:A:89:PRO:HD2	1.67	0.42
1:A:332:LYS:C	1:A:334:GLY:N	2.77	0.42
1:A:1239:ARG:C	1:A:1240:CYS:SG	3.01	0.42
1:A:1279:ILE:O	1:A:1279:ILE:HG22	2.18	0.42
2:B:26:THR:O	2:B:29:ASP:N	2.51	0.42
2:B:309:GLN:OE1	7:I:52:ILE:HG23	2.19	0.42
2:B:523:CYS:SG	2:B:750:GLY:N	2.92	0.42
2:B:701:ILE:HG21	2:B:740:HIS:CE1	2.52	0.42
2:B:766:ARG:HA	2:B:766:ARG:HD3	1.90	0.42
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	2.02	0.42
3:C:29:MET:HB3	9:K:45:LEU:CD1	2.49	0.42
4:E:198:ILE:CD1	4:E:212:ARG:HG2	2.43	0.42
1:A:402:ALA:HB1	1:A:434:ARG:HA	2.01	0.42
1:A:692:ASP:HA	1:A:695:LYS:HB2	2.01	0.42
2:B:314:LEU:O	2:B:315:LYS:C	2.63	0.42
2:B:377:PHE:O	2:B:380:TYR:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:LEU:O	2:B:382:ILE:HG12	2.20	0.42
2:B:1077:THR:HG21	2:B:1079:LYS:HB2	2.01	0.42
3:C:99:LEU:HD13	3:C:120:ILE:HA	2.01	0.42
3:C:167:HIS:CD2	3:C:167:HIS:C	2.97	0.42
4:E:21:GLU:HG3	4:E:35:VAL:HG21	2.02	0.42
4:E:28:TYR:CE1	4:E:78:LEU:CD1	2.95	0.42
6:H:93:TYR:HB3	6:H:144:ILE:O	2.19	0.42
7:I:30:ARG:HE	7:I:30:ARG:HB3	1.70	0.42
10:L:61:THR:HG22	10:L:63:ARG:N	2.34	0.42
1:A:1153:TYR:CE1	7:I:42:LEU:HD13	2.55	0.42
2:B:638:PHE:HB2	2:B:741:CYS:O	2.19	0.42
3:C:31:ASN:O	3:C:33:LEU:N	2.52	0.42
5:F:85:MET:CE	5:F:148:VAL:HG13	2.49	0.42
6:H:107:VAL:HG21	6:H:126:GLU:HG3	2.02	0.42
9:K:65:HIS:C	9:K:67:PHE:N	2.75	0.42
1:A:873:MET:HB3	1:A:878:ILE:HD11	2.01	0.42
2:B:612:GLU:O	2:B:632:ARG:NH2	2.52	0.42
2:B:784:ASN:HD21	2:B:788:ARG:HD3	1.85	0.42
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.54	0.42
2:B:886:LYS:HB2	2:B:890:TYR:CZ	2.54	0.42
2:B:1084:GLN:OE1	2:B:1084:GLN:N	2.49	0.42
3:C:204:SER:O	3:C:206:ASN:N	2.53	0.42
7:I:53:GLY:C	7:I:90:GLN:HB2	2.44	0.42
8:J:23:ASN:C	8:J:25:LEU:N	2.77	0.42
9:K:91:CYS:O	9:K:95:ILE:HG12	2.19	0.42
1:A:30:ILE:HG12	2:B:1170:THR:CG2	2.49	0.42
1:A:341:MET:HB3	1:A:341:MET:HE3	1.76	0.42
1:A:345:VAL:HG12	2:B:1155:SER:HB2	2.00	0.42
1:A:504:LEU:N	1:A:504:LEU:CD1	2.82	0.42
1:A:550:LEU:HD12	1:A:556:TRP:NE1	2.35	0.42
1:A:1006:ILE:HG12	1:A:1007:ILE:N	2.33	0.42
1:A:1062:GLU:OE1	1:A:1067:LEU:HD13	2.19	0.42
1:A:1209:MET:CE	1:A:1228:TRP:HB2	2.50	0.42
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.20	0.42
2:B:814:PHE:C	2:B:816:GLU:H	2.28	0.42
2:B:1072:MET:HE3	2:B:1085:ILE:HD13	2.00	0.42
3:C:47:ASP:HB3	3:C:160:LYS:HD2	2.00	0.42
1:A:549:MET:HA	1:A:552:TRP:HB2	2.02	0.42
1:A:583:PRO:O	1:A:610:GLY:CA	2.68	0.42
1:A:779:PHE:CZ	2:B:517:THR:HA	2.55	0.42
1:A:894:GLU:O	1:A:896:ARG:N	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:VAL:HG13	1:A:1052:GLN:HB3	2.01	0.42
1:A:1002:GLY:HA3	1:A:1007:ILE:HG21	2.02	0.42
1:A:1326:ARG:O	1:A:1327:ILE:C	2.63	0.42
2:B:309:GLN:O	2:B:310:MET:C	2.63	0.42
2:B:780:VAL:HA	2:B:795:ILE:HG22	2.01	0.42
2:B:1150:ARG:HD3	2:B:1150:ARG:HA	1.86	0.42
1:A:15:LYS:HB3	2:B:1220:ARG:HD3	2.02	0.41
1:A:77:CYS:HA	1:A:78:PRO:HD3	1.91	0.41
1:A:384:ASN:O	1:A:385:ILE:C	2.63	0.41
1:A:482:PHE:CE1	2:B:836:GLU:HB2	2.55	0.41
1:A:884:ASP:OD2	1:A:884:ASP:N	2.51	0.41
1:A:1189:SER:O	1:A:1241:ARG:HD3	2.20	0.41
2:B:202:TYR:CD1	2:B:209:GLU:HG2	2.55	0.41
2:B:350:GLN:O	2:B:351:TYR:C	2.62	0.41
2:B:1159:ARG:HD3	2:B:1193:GLN:HE21	1.85	0.41
1:A:451:HIS:O	2:B:1137:CYS:SG	2.77	0.41
1:A:652:VAL:O	1:A:655:PHE:N	2.53	0.41
1:A:1163:ILE:H	1:A:1163:ILE:HG13	1.74	0.41
1:A:1325:THR:HA	4:E:147:HIS:HA	2.01	0.41
1:A:1436:ILE:HG22	1:A:1437:GLY:N	2.33	0.41
2:B:190:TYR:OH	2:B:196:PRO:HG3	2.20	0.41
2:B:762:ASN:HD22	2:B:762:ASN:HA	1.58	0.41
2:B:805:THR:CB	2:B:815:ARG:HH21	2.32	0.41
8:J:42:LYS:HE3	8:J:43:ARG:NH2	2.35	0.41
8:J:48:ARG:HE	8:J:49:MET:HE2	1.85	0.41
1:A:56:PRO:O	1:A:57:ARG:CG	2.64	0.41
1:A:405:VAL:O	1:A:413:ILE:HB	2.20	0.41
1:A:432:VAL:O	1:A:433:GLU:C	2.63	0.41
1:A:1038:THR:O	1:A:1041:ALA:N	2.54	0.41
2:B:31:TRP:CD1	2:B:807:ARG:NH1	2.88	0.41
2:B:803:LEU:HD22	2:B:1035:ALA:CB	2.50	0.41
2:B:978:ASP:HB2	2:B:980:PHE:HE1	1.82	0.41
3:C:181:ASP:HA	3:C:182:PRO:HD2	1.79	0.41
3:C:232:VAL:HG21	3:C:244:VAL:HG12	2.02	0.41
4:E:127:ILE:HD13	4:E:127:ILE:H	1.84	0.41
5:F:94:LEU:HD22	5:F:122:MET:HG2	2.01	0.41
9:K:36:GLU:HB3	9:K:37:LYS:HG2	2.00	0.41
2:B:463:THR:HG23	12:T:26:DA:H4'	2.02	0.41
2:B:597:MET:SD	2:B:624:LEU:HD11	2.61	0.41
2:B:957:ASN:HD22	2:B:957:ASN:C	2.29	0.41
3:C:44:LEU:HD12	3:C:160:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:105:GLY:HA3	3:C:149:LYS:O	2.19	0.41
6:H:26:ILE:HG23	6:H:26:ILE:O	2.21	0.41
7:I:46:HIS:O	7:I:47:GLU:HB2	2.20	0.41
7:I:62:ILE:C	7:I:64:SER:H	2.28	0.41
9:K:50:LEU:HD23	9:K:56:VAL:HG11	2.01	0.41
1:A:68:GLN:OE1	1:A:68:GLN:O	2.38	0.41
1:A:269:ILE:HG23	1:A:299:HIS:HB2	2.01	0.41
1:A:456:MET:HG2	1:A:478:TYR:OH	2.20	0.41
1:A:568:PRO:HD3	6:H:94:ASP:O	2.19	0.41
1:A:783:THR:O	1:A:784:LEU:HD23	2.21	0.41
1:A:964:ILE:HA	1:A:964:ILE:HD13	1.83	0.41
1:A:1004:ASN:CG	4:E:167:ARG:HD3	2.45	0.41
2:B:44:VAL:O	2:B:47:GLN:N	2.53	0.41
2:B:173:MET:HB3	2:B:176:SER:HB3	2.02	0.41
2:B:597:MET:O	2:B:598:GLU:C	2.64	0.41
2:B:739:THR:OG1	2:B:740:HIS:N	2.53	0.41
2:B:902:GLY:O	2:B:948:ILE:HG23	2.20	0.41
2:B:1060:ARG:NH1	3:C:199:LYS:O	2.47	0.41
3:C:258:ILE:HG13	9:K:35:PHE:HE2	1.84	0.41
5:F:103:MET:C	5:F:104:ASN:ND2	2.78	0.41
1:A:829:VAL:O	1:A:831:THR:N	2.53	0.41
1:A:962:ARG:C	1:A:964:ILE:H	2.29	0.41
2:B:34:ILE:CG1	2:B:542:MET:HE1	2.49	0.41
2:B:470:LYS:C	2:B:472:ALA:H	2.29	0.41
2:B:763:GLN:HG2	2:B:765:PRO:HD2	2.02	0.41
2:B:973:ILE:HA	2:B:974:PRO:HD3	1.89	0.41
5:F:111:LEU:C	5:F:113:GLY:H	2.28	0.41
1:A:11:LEU:HD11	2:B:1195:HIS:HD2	1.85	0.41
1:A:167:CYS:O	1:A:167:CYS:SG	2.77	0.41
1:A:451:HIS:CE1	1:A:1074:GLU:HG3	2.56	0.41
1:A:841:LEU:HA	1:A:841:LEU:HD23	1.84	0.41
1:A:845:LEU:O	1:A:846:GLU:C	2.64	0.41
1:A:858:ASN:O	1:A:861:GLY:N	2.45	0.41
1:A:892:ALA:O	1:A:896:ARG:HB2	2.21	0.41
1:A:983:ILE:O	1:A:983:ILE:CG2	2.68	0.41
2:B:229:ALA:HB1	2:B:231:PRO:HD2	2.03	0.41
2:B:637:LEU:HD22	2:B:741:CYS:O	2.20	0.41
2:B:1066:SER:C	2:B:1067:ARG:HD2	2.45	0.41
2:B:1160:VAL:O	2:B:1194:ILE:HD13	2.21	0.41
3:C:99:LEU:HD11	3:C:120:ILE:HD13	2.02	0.41
6:H:95:TYR:HB3	6:H:144:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:53:ASP:O	9:K:56:VAL:HG22	2.21	0.41
11:R:8:G:N2	12:T:21:DT:H1'	2.35	0.41
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.89	0.41
1:A:1062:GLU:N	5:F:88:TYR:HE1	2.19	0.41
1:A:1316:VAL:O	1:A:1319:VAL:HB	2.20	0.41
2:B:360:PHE:HD2	2:B:374:LYS:HD3	1.85	0.41
2:B:999:MET:HG3	2:B:1008:PRO:HD2	2.02	0.41
3:C:82:TYR:CE2	3:C:84:ARG:NH2	2.88	0.41
4:E:61:GLN:HG2	4:E:62:ALA:N	2.36	0.41
5:F:111:LEU:CD1	5:F:111:LEU:N	2.83	0.41
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.54	0.41
1:A:179:LEU:HD13	1:A:301:ALA:HB2	2.02	0.41
1:A:306:ASN:N	1:A:306:ASN:HD22	2.18	0.41
1:A:350:ARG:HB3	2:B:1128:LEU:HD11	2.03	0.41
1:A:350:ARG:NH2	12:T:21:DT:H2''	2.35	0.41
1:A:412:ARG:C	1:A:413:ILE:HD12	2.45	0.41
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.56	0.41
1:A:746:MET:HE1	2:B:1018:PRO:HG3	2.03	0.41
1:A:754:SER:OG	1:A:757:ASN:ND2	2.54	0.41
1:A:802:ASN:ND2	2:B:728:ARG:HB2	2.35	0.41
1:A:814:PHE:O	1:A:817:ALA:HB3	2.20	0.41
1:A:903:ASN:O	1:A:907:THR:OG1	2.37	0.41
1:A:1152:ILE:HD13	7:I:44:TYR:HD2	1.85	0.41
1:A:1154:TYR:HD2	7:I:25:LEU:HD22	1.86	0.41
1:A:1263:ILE:CG2	1:A:1264:GLU:N	2.83	0.41
1:A:1398:MET:C	1:A:1400:CYS:N	2.77	0.41
1:A:1425:SER:O	1:A:1427:ASN:N	2.54	0.41
2:B:522:VAL:CG1	2:B:537:LYS:HB2	2.51	0.41
2:B:681:TRP:CH2	2:B:690:VAL:HG11	2.56	0.41
3:C:90:ASP:HB3	3:C:91:HIS:H	1.78	0.41
3:C:181:ASP:OD1	3:C:185:LYS:HG2	2.20	0.41
4:E:99:HIS:CD2	4:E:99:HIS:C	2.99	0.41
5:F:82:THR:HG22	5:F:84:TYR:HB2	2.03	0.41
5:F:152:ILE:H	5:F:152:ILE:HD12	1.86	0.41
7:I:14:LEU:CD2	7:I:29:CYS:HB2	2.51	0.41
7:I:78:CYS:SG	7:I:105:SER:HB2	2.61	0.41
8:J:57:ILE:HA	8:J:60:PHE:CD2	2.47	0.41
9:K:31:VAL:O	9:K:74:ARG:HA	2.20	0.41
1:A:315:LEU:CD1	1:A:319:GLY:HA2	2.51	0.41
1:A:379:VAL:HG12	1:A:380:VAL:H	1.86	0.41
1:A:556:TRP:CD1	1:A:557:ASP:H	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ARG:O	1:A:591:PHE:HB2	2.21	0.41
1:A:619:LYS:O	1:A:623:GLY:HA3	2.20	0.41
1:A:666:ILE:HG23	2:B:1026:LEU:CB	2.50	0.41
2:B:301:ILE:HA	2:B:379:GLY:O	2.21	0.41
2:B:553:PRO:HA	2:B:556:THR:HG22	2.03	0.41
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.56	0.41
2:B:578:THR:OG1	2:B:593:PRO:HG3	2.21	0.41
2:B:710:LEU:HD23	2:B:710:LEU:HA	1.77	0.41
2:B:728:ARG:NH1	2:B:760:ASP:OD2	2.54	0.41
2:B:795:ILE:HD11	2:B:854:LEU:HB2	2.03	0.41
2:B:1045:SER:HA	2:B:1046:PRO:HD3	1.87	0.41
4:E:112:TYR:CZ	4:E:116:ILE:HD11	2.55	0.41
4:E:112:TYR:O	4:E:137:GLU:HG2	2.21	0.41
6:H:89:LEU:HD13	6:H:91:ASP:CG	2.45	0.41
7:I:55:THR:HG23	7:I:55:THR:O	2.21	0.41
7:I:68:LEU:HB3	7:I:84:VAL:HG22	2.01	0.41
1:A:9:ALA:HA	1:A:10:PRO:HD3	1.90	0.40
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.86	0.40
1:A:909:ASP:CG	1:A:911:SER:HB3	2.45	0.40
2:B:190:TYR:HD2	8:J:63:TYR:CD2	2.38	0.40
2:B:310:MET:O	2:B:313:MET:HB2	2.20	0.40
2:B:464:GLY:C	2:B:478:GLY:HA2	2.47	0.40
2:B:884:ARG:O	2:B:936:ASP:HB3	2.21	0.40
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.22	0.40
4:E:89:GLY:O	4:E:91:LYS:N	2.54	0.40
5:F:81:THR:O	5:F:136:ARG:NH1	2.54	0.40
1:A:31:SER:OG	1:A:83:HIS:CD2	2.75	0.40
1:A:106:VAL:HG12	1:A:107:CYS:H	1.86	0.40
1:A:399:HIS:O	1:A:435:HIS:CD2	2.74	0.40
1:A:714:PHE:CD2	7:I:97:MET:HE1	2.57	0.40
1:A:964:ILE:CD1	1:A:1037:LEU:HD21	2.47	0.40
1:A:1341:ILE:CD1	1:A:1379:GLY:O	2.69	0.40
2:B:57:TYR:O	2:B:60:GLN:HB3	2.21	0.40
2:B:778:MET:HE3	2:B:1094:ARG:HG2	2.03	0.40
6:H:31:THR:O	6:H:32:THR:OG1	2.30	0.40
1:A:299:HIS:HA	1:A:302:THR:HB	2.03	0.40
1:A:765:VAL:CG2	1:A:800:VAL:CB	2.86	0.40
1:A:794:PRO:HG2	1:A:795:GLU:H	1.85	0.40
1:A:1059:HIS:HB3	5:F:86:THR:HB	2.03	0.40
2:B:485:ARG:CZ	2:B:782:LEU:HD11	2.52	0.40
2:B:803:LEU:HD22	2:B:1035:ALA:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:861:ASP:OD1	2:B:862:GLN:N	2.55	0.40
3:C:234:SER:HB3	3:C:240:VAL:HG23	2.03	0.40
6:H:94:ASP:OD1	6:H:94:ASP:N	2.55	0.40
7:I:26:LEU:HD13	7:I:35:VAL:HG11	2.02	0.40
1:A:265:LYS:HZ2	1:A:323:LYS:HG2	1.87	0.40
1:A:320:ARG:HG3	2:B:471:LYS:HG2	2.04	0.40
1:A:526:ASP:O	1:A:527:THR:C	2.63	0.40
1:A:795:GLU:H	1:A:795:GLU:HG3	1.48	0.40
1:A:1064:VAL:HG12	1:A:1370:LEU:HD22	2.02	0.40
2:B:600:LEU:O	2:B:601:ARG:C	2.65	0.40
2:B:610:ASN:OD1	2:B:610:ASN:C	2.64	0.40
2:B:642:ASP:OD2	2:B:649:LYS:NZ	2.55	0.40
2:B:910:VAL:HG12	2:B:911:ILE:H	1.85	0.40
2:B:979:LYS:HE3	2:B:1095:LEU:HD12	2.02	0.40
2:B:994:TYR:HB2	2:B:999:MET:HE1	2.02	0.40
1:A:870:GLU:HG3	4:E:208:TYR:CG	2.57	0.40
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.69	0.40
1:A:1004:ASN:OD1	1:A:1004:ASN:C	2.64	0.40
1:A:1017:LEU:HB2	4:E:205:SER:HA	2.03	0.40
1:A:1350:LYS:O	1:A:1354:ASN:HB2	2.22	0.40
1:A:1404:GLU:C	1:A:1407:GLU:OE2	2.65	0.40
1:A:1424:VAL:O	1:A:1425:SER:C	2.65	0.40
2:B:228:LYS:NZ	2:B:234:ILE:HG13	2.36	0.40
2:B:289:LEU:HD23	2:B:289:LEU:HA	1.95	0.40
2:B:384:ARG:HH12	2:B:621:GLU:CD	2.30	0.40
2:B:1024:ALA:O	2:B:1025:HIS:C	2.64	0.40
4:E:147:HIS:HB3	4:E:150:VAL:HG23	2.02	0.40
5:F:82:THR:HG22	5:F:84:TYR:H	1.86	0.40
8:J:25:LEU:HA	8:J:25:LEU:HD23	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1383/1733 (80%)	1075 (78%)	218 (16%)	90 (6%)	1	14
2	B	1088/1224 (89%)	849 (78%)	169 (16%)	70 (6%)	1	14
3	C	264/318 (83%)	211 (80%)	39 (15%)	14 (5%)	1	16
4	E	212/215 (99%)	177 (84%)	31 (15%)	4 (2%)	6	32
5	F	82/155 (53%)	73 (89%)	6 (7%)	3 (4%)	2	21
6	H	129/146 (88%)	96 (74%)	20 (16%)	13 (10%)	0	7
7	I	117/122 (96%)	92 (79%)	18 (15%)	7 (6%)	1	14
8	J	63/70 (90%)	48 (76%)	11 (18%)	4 (6%)	1	14
9	K	112/120 (93%)	95 (85%)	15 (13%)	2 (2%)	6	33
10	L	44/70 (63%)	32 (73%)	9 (20%)	3 (7%)	1	12
All	All	3494/4173 (84%)	2748 (79%)	536 (15%)	210 (6%)	1	14

All (210) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	PRO
1	A	93	VAL
1	A	226	GLU
1	A	253	ASN
1	A	254	GLU
1	A	258	GLY
1	A	312	PRO
1	A	313	GLN
1	A	317	LYS
1	A	321	PRO
1	A	325	ILE
1	A	424	ILE
1	A	517	ASN
1	A	567	LYS
1	A	597	LEU
1	A	830	LYS
1	A	846	GLU
1	A	889	SER
1	A	972	HIS
1	A	998	LEU
1	A	1261	LYS
1	A	1365	TYR
1	A	1435	PRO
2	B	21	GLU

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Mol	Chain	Res	Type
2	B	67	SER
2	B	176	SER
2	B	223	VAL
2	B	229	ALA
2	B	249	ARG
2	B	466	TRP
2	B	477	ALA
2	B	479	VAL
2	B	480	SER
2	B	483	LEU
2	B	563	MET
2	B	636	PRO
2	B	643	ASP
2	B	731	VAL
2	B	735	ALA
2	B	738	PHE
2	B	809	MET
2	B	864	LYS
2	B	903	VAL
2	B	958	GLN
2	B	1066	SER
2	B	1155	SER
2	B	1176	ASN
2	B	1178	ASN
2	B	1183	LYS
4	E	90	VAL
5	F	104	ASN
6	H	32	THR
6	H	61	SER
6	H	78	SER
6	H	82	PRO
6	H	140	ALA
7	I	33	SER
7	I	54	GLU
8	J	2	ILE
8	J	6	ARG
10	L	46	VAL
1	A	46	THR
1	A	50	ILE
1	A	55	ASP
1	A	68	GLN
1	A	86	LEU

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Mol	Chain	Res	Type
1	A	89	PRO
1	A	178	GLY
1	A	257	ARG
1	A	266	LEU
1	A	315	LEU
1	A	538	ASP
1	A	543	LEU
1	A	628	GLY
1	A	774	ARG
1	A	821	ARG
1	A	859	SER
1	A	958	VAL
1	A	1221	LYS
1	A	1229	SER
1	A	1437	GLY
2	B	100	PRO
2	B	200	GLY
2	B	265	SER
2	B	365	THR
2	B	436	VAL
2	B	450	ALA
2	B	475	SER
2	B	488	TYR
2	B	709	ASP
2	B	837	ASP
2	B	901	PRO
2	B	976	ILE
2	B	1082	MET
2	B	1096	ARG
2	B	1126	GLY
2	B	1131	GLY
2	B	1156	ASP
3	C	110	THR
3	C	212	PRO
4	E	192	ARG
5	F	82	THR
6	H	108	SER
6	H	129	TYR
7	I	76	PRO
9	K	81	TYR
10	L	56	LEU
1	A	48	ALA

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Mol	Chain	Res	Type
1	A	202	LEU
1	A	251	SER
1	A	333	GLU
1	A	576	GLN
1	A	895	LYS
2	B	45	SER
2	B	121	ASN
2	B	266	ALA
2	B	307	ASP
2	B	468	GLU
2	B	734	HIS
2	B	869	SER
3	C	167	HIS
4	E	59	SER
5	F	112	GLU
6	H	52	GLN
7	I	34	TYR
7	I	47	GLU
7	I	88	SER
8	J	29	GLU
1	A	72	GLU
1	A	308	ILE
1	A	314	ALA
1	A	418	SER
1	A	454	SER
1	A	465	TYR
1	A	1016	THR
1	A	1270	ASN
2	B	248	SER
2	B	322	PHE
2	B	454	THR
2	B	549	THR
2	B	699	GLU
2	B	724	ASP
2	B	974	PRO
2	B	1116	ARG
2	B	1153	GLU
2	B	1157	ALA
3	C	28	ALA
3	C	142	VAL
3	C	144	ILE
3	C	214	ASN

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Mol	Chain	Res	Type
6	H	3	ASN
10	L	42	ARG
1	A	40	THR
1	A	63	ARG
1	A	130	ASP
1	A	248	PRO
1	A	324	SER
1	A	332	LYS
1	A	385	ILE
1	A	386	ASP
1	A	404	TYR
1	A	525	GLN
1	A	639	PRO
1	A	896	ARG
1	A	933	TYR
1	A	1062	GLU
1	A	1280	GLU
1	A	1384	VAL
1	A	1393	ASN
2	B	359	GLU
2	B	370	PHE
2	B	467	GLY
2	B	792	MET
2	B	1211	ASN
3	C	6	PRO
3	C	172	PRO
3	C	213	PRO
3	C	227	THR
3	C	265	MET
4	E	124	VAL
6	H	62	SER
6	H	92	ASP
6	H	135	LEU
9	K	10	PHE
1	A	149	GLU
1	A	399	HIS
1	A	492	PRO
1	A	886	ILE
1	A	1424	VAL
2	B	876	LYS
2	B	1214	PRO
3	C	253	LYS

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Mol	Chain	Res	Type
7	I	21	GLU
1	A	168	GLY
1	A	667	GLY
1	A	986	ILE
1	A	250	ILE
1	A	946	VAL
1	A	1146	VAL
2	B	611	PRO
2	B	1046	PRO
3	C	240	VAL
1	A	166	GLY
1	A	1327	ILE
6	H	85	GLY
1	A	1388	GLY
2	B	301	ILE
8	J	64	ASN
1	A	35	ILE
1	A	583	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1218/1520 (80%)	974 (80%)	244 (20%)	1	8
2	B	960/1061 (90%)	775 (81%)	185 (19%)	1	9
3	C	234/274 (85%)	181 (77%)	53 (23%)	1	5
4	E	196/197 (100%)	172 (88%)	24 (12%)	5	21
5	F	74/137 (54%)	64 (86%)	10 (14%)	4	19
6	H	117/128 (91%)	99 (85%)	18 (15%)	2	15
7	I	113/116 (97%)	89 (79%)	24 (21%)	1	6
8	J	60/65 (92%)	49 (82%)	11 (18%)	2	11
9	K	99/102 (97%)	83 (84%)	16 (16%)	2	14
10	L	40/57 (70%)	35 (88%)	5 (12%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3111/3657 (85%)	2521 (81%)	590 (19%)	1 10

All (590) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	12	ARG
1	A	13	THR
1	A	14	VAL
1	A	26	GLU
1	A	32	VAL
1	A	40	THR
1	A	44	THR
1	A	47	ARG
1	A	49	LYS
1	A	58	LEU
1	A	68	GLN
1	A	70	CYS
1	A	71	GLN
1	A	81	PHE
1	A	84	ILE
1	A	88	LYS
1	A	93	VAL
1	A	99	ILE
1	A	102	VAL
1	A	105	CYS
1	A	113	LEU
1	A	114	LEU
1	A	115	LEU
1	A	126	LEU
1	A	144	THR
1	A	147	VAL
1	A	149	GLU
1	A	169	ASN
1	A	186	LYS
1	A	216	VAL
1	A	222	LEU
1	A	225	ASN
1	A	230	ARG
1	A	235	ILE
1	A	250	ILE
1	A	252	PHE

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Mol	Chain	Res	Type
1	A	259	GLU
1	A	263	THR
1	A	269	ILE
1	A	271	LYS
1	A	274	ILE
1	A	276	LEU
1	A	287	HIS
1	A	289	ILE
1	A	304	MET
1	A	306	ASN
1	A	308	ILE
1	A	313	GLN
1	A	318	SER
1	A	320	ARG
1	A	322	VAL
1	A	323	LYS
1	A	325	ILE
1	A	329	LEU
1	A	332	LYS
1	A	336	ILE
1	A	337	ARG
1	A	340	LEU
1	A	362	ASP
1	A	368	LYS
1	A	379	VAL
1	A	385	ILE
1	A	388	LEU
1	A	397	ASN
1	A	403	LYS
1	A	406	ILE
1	A	411	ASP
1	A	412	ARG
1	A	419	LYS
1	A	424	ILE
1	A	431	LYS
1	A	436	ILE
1	A	438	ASP
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	452	LYS
1	A	453	MET

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Mol	Chain	Res	Type
1	A	456	MET
1	A	463	ILE
1	A	466	SER
1	A	469	ARG
1	A	472	LEU
1	A	475	THR
1	A	476	SER
1	A	481	ASP
1	A	493	GLN
1	A	494	SER
1	A	496	GLU
1	A	501	LEU
1	A	516	SER
1	A	518	LYS
1	A	521	MET
1	A	525	GLN
1	A	531	ILE
1	A	534	LEU
1	A	535	THR
1	A	536	LEU
1	A	541	ILE
1	A	550	LEU
1	A	557	ASP
1	A	565	ILE
1	A	567	LYS
1	A	572	TRP
1	A	576	GLN
1	A	577	ILE
1	A	596	THR
1	A	597	LEU
1	A	599	SER
1	A	617	VAL
1	A	618	GLU
1	A	630	ILE
1	A	634	THR
1	A	635	ARG
1	A	658	LEU
1	A	660	ASN
1	A	662	PHE
1	A	664	THR
1	A	666	ILE
1	A	675	THR

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Mol	Chain	Res	Type
1	A	677	ARG
1	A	680	THR
1	A	691	LEU
1	A	694	THR
1	A	695	LYS
1	A	731	ARG
1	A	740	LEU
1	A	741	ASN
1	A	747	VAL
1	A	756	ILE
1	A	764	CYS
1	A	768	GLN
1	A	769	SER
1	A	782	ARG
1	A	783	THR
1	A	795	GLU
1	A	800	VAL
1	A	801	GLU
1	A	805	LEU
1	A	806	ARG
1	A	808	LEU
1	A	826	ASP
1	A	829	VAL
1	A	830	LYS
1	A	850	VAL
1	A	858	ASN
1	A	863	VAL
1	A	867	ILE
1	A	870	GLU
1	A	882	SER
1	A	884	ASP
1	A	885	THR
1	A	896	ARG
1	A	898	ARG
1	A	902	LEU
1	A	907	THR
1	A	911	SER
1	A	915	SER
1	A	918	GLU
1	A	920	LEU
1	A	938	LYS
1	A	949	ASP

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Mol	Chain	Res	Type
1	A	958	VAL
1	A	962	ARG
1	A	964	ILE
1	A	977	LYS
1	A	988	LEU
1	A	990	VAL
1	A	993	LEU
1	A	996	ASN
1	A	999	VAL
1	A	1000	LEU
1	A	1004	ASN
1	A	1006	ILE
1	A	1017	LEU
1	A	1020	CYS
1	A	1022	LEU
1	A	1025	ARG
1	A	1032	LEU
1	A	1033	GLN
1	A	1043	ASP
1	A	1049	ILE
1	A	1058	VAL
1	A	1067	LEU
1	A	1077	THR
1	A	1080	THR
1	A	1095	THR
1	A	1116	LEU
1	A	1118	VAL
1	A	1120	LEU
1	A	1128	GLN
1	A	1135	ARG
1	A	1142	THR
1	A	1146	VAL
1	A	1152	ILE
1	A	1163	ILE
1	A	1187	GLN
1	A	1193	LEU
1	A	1219	THR
1	A	1226	VAL
1	A	1232	ASN
1	A	1237	ILE
1	A	1239	ARG
1	A	1240	CYS

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Mol	Chain	Res	Type
1	A	1242	VAL
1	A	1262	LYS
1	A	1263	ILE
1	A	1264	GLU
1	A	1271	ILE
1	A	1279	ILE
1	A	1280	GLU
1	A	1282	VAL
1	A	1283	VAL
1	A	1284	MET
1	A	1291	VAL
1	A	1295	THR
1	A	1299	VAL
1	A	1308	THR
1	A	1309	ASP
1	A	1322	ILE
1	A	1325	THR
1	A	1329	THR
1	A	1333	ILE
1	A	1335	ILE
1	A	1336	MET
1	A	1345	ARG
1	A	1350	LYS
1	A	1351	GLU
1	A	1354	ASN
1	A	1372	VAL
1	A	1376	THR
1	A	1377	THR
1	A	1378	GLN
1	A	1385	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1394	THR
1	A	1407	GLU
1	A	1420	ASP
1	A	1425	SER
1	A	1428	VAL
1	A	1436	ILE
1	A	1445	ILE
2	B	25	ILE
2	B	26	THR
2	B	28	GLU

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Mol	Chain	Res	Type
2	B	34	ILE
2	B	43	LEU
2	B	45	SER
2	B	46	GLN
2	B	57	TYR
2	B	61	ASP
2	B	63	ILE
2	B	65	GLU
2	B	68	THR
2	B	90	ILE
2	B	97	VAL
2	B	98	THR
2	B	102	VAL
2	B	104	GLU
2	B	108	VAL
2	B	120	ARG
2	B	131	ASP
2	B	132	VAL
2	B	134	LYS
2	B	167	ILE
2	B	169	ARG
2	B	174	LEU
2	B	175	ARG
2	B	189	LEU
2	B	194	GLU
2	B	199	MET
2	B	202	TYR
2	B	217	ARG
2	B	222	ILE
2	B	223	VAL
2	B	225	VAL
2	B	234	ILE
2	B	239	GLU
2	B	240	ILE
2	B	244	LEU
2	B	246	LYS
2	B	249	ARG
2	B	254	LEU
2	B	268	THR
2	B	273	LEU
2	B	276	ILE
2	B	294	ASP

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Mol	Chain	Res	Type
2	B	296	GLU
2	B	298	LEU
2	B	305	VAL
2	B	313	MET
2	B	314	LEU
2	B	327	ARG
2	B	347	LYS
2	B	349	ILE
2	B	359	GLU
2	B	361	LEU
2	B	387	LEU
2	B	388	CYS
2	B	393	LYS
2	B	403	LYS
2	B	404	LYS
2	B	416	LEU
2	B	418	LYS
2	B	423	LYS
2	B	425	THR
2	B	429	PHE
2	B	453	ILE
2	B	459	TYR
2	B	463	THR
2	B	471	LYS
2	B	474	SER
2	B	481	GLN
2	B	482	VAL
2	B	483	LEU
2	B	485	ARG
2	B	493	SER
2	B	513	GLN
2	B	516	ASN
2	B	527	THR
2	B	529	GLU
2	B	537	LYS
2	B	545	ILE
2	B	547	VAL
2	B	552	MET
2	B	559	SER
2	B	563	MET
2	B	567	GLU
2	B	570	VAL

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Mol	Chain	Res	Type
2	B	576	ASP
2	B	613	VAL
2	B	616	ILE
2	B	619	ILE
2	B	622	LYS
2	B	637	LEU
2	B	638	PHE
2	B	642	ASP
2	B	643	ASP
2	B	653	VAL
2	B	655	LYS
2	B	658	ILE
2	B	661	LEU
2	B	664	THR
2	B	678	GLU
2	B	680	THR
2	B	682	SER
2	B	694	ASP
2	B	701	ILE
2	B	702	LEU
2	B	703	ILE
2	B	705	MET
2	B	708	GLU
2	B	709	ASP
2	B	710	LEU
2	B	730	ARG
2	B	731	VAL
2	B	737	THR
2	B	740	HIS
2	B	754	SER
2	B	755	ILE
2	B	762	ASN
2	B	771	SER
2	B	773	MET
2	B	788	ARG
2	B	791	THR
2	B	792	MET
2	B	795	ILE
2	B	796	LEU
2	B	801	LYS
2	B	817	LEU
2	B	824	ILE

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Mol	Chain	Res	Type
2	B	831	SER
2	B	839	MET
2	B	840	ILE
2	B	844	SER
2	B	857	ARG
2	B	865	LYS
2	B	873	THR
2	B	878	GLN
2	B	882	THR
2	B	884	ARG
2	B	886	LYS
2	B	889	THR
2	B	894	ASP
2	B	915	THR
2	B	970	THR
2	B	971	THR
2	B	995	ARG
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1010	LEU
2	B	1013	ASN
2	B	1020	ARG
2	B	1048	THR
2	B	1051	THR
2	B	1059	LEU
2	B	1062	HIS
2	B	1067	ARG
2	B	1072	MET
2	B	1081	LEU
2	B	1084	GLN
2	B	1095	LEU
2	B	1099	VAL
2	B	1113	VAL
2	B	1114	LEU
2	B	1115	THR
2	B	1120	GLU
2	B	1122	ARG
2	B	1123	SER
2	B	1132	GLU
2	B	1138	MET

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Mol	Chain	Res	Type
2	B	1159	ARG
2	B	1166	CYS
2	B	1170	THR
2	B	1172	ILE
2	B	1177	HIS
2	B	1178	ASN
2	B	1183	LYS
2	B	1191	ILE
2	B	1194	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1203	LEU
2	B	1207	LEU
2	B	1211	ASN
3	C	3	GLU
3	C	4	GLU
3	C	10	ILE
3	C	15	LYS
3	C	18	VAL
3	C	24	ASN
3	C	26	ASP
3	C	27	LEU
3	C	33	LEU
3	C	37	MET
3	C	40	GLU
3	C	43	THR
3	C	53	THR
3	C	54	ASN
3	C	56	THR
3	C	57	VAL
3	C	60	ASP
3	C	61	GLU
3	C	66	ARG
3	C	77	ILE
3	C	81	GLU
3	C	89	GLU
3	C	90	ASP
3	C	99	LEU
3	C	111	THR
3	C	116	LYS
3	C	120	ILE
3	C	129	ILE

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Mol	Chain	Res	Type
3	C	134	ILE
3	C	138	GLU
3	C	140	ASN
3	C	143	LEU
3	C	147	LEU
3	C	148	ARG
3	C	149	LYS
3	C	155	LEU
3	C	156	THR
3	C	163	ILE
3	C	166	GLU
3	C	178	PHE
3	C	183	TRP
3	C	185	LYS
3	C	224	GLN
3	C	226	ASP
3	C	233	GLU
3	C	235	VAL
3	C	237	SER
3	C	240	VAL
3	C	244	VAL
3	C	248	ILE
3	C	258	ILE
3	C	266	ASP
3	C	267	GLN
4	E	3	GLN
4	E	31	THR
4	E	32	GLN
4	E	61	GLN
4	E	65	THR
4	E	72	PHE
4	E	83	CYS
4	E	88	VAL
4	E	94	LYS
4	E	103	LYS
4	E	107	THR
4	E	127	ILE
4	E	134	THR
4	E	150	VAL
4	E	158	SER
4	E	166	LYS
4	E	169	ARG

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Mol	Chain	Res	Type
4	E	184	VAL
4	E	187	TYR
4	E	190	LEU
4	E	198	ILE
4	E	200	ARG
4	E	201	LYS
4	E	212	ARG
5	F	77	ASP
5	F	81	THR
5	F	90	ARG
5	F	97	ARG
5	F	104	ASN
5	F	111	LEU
5	F	112	GLU
5	F	120	ILE
5	F	123	LYS
5	F	155	LEU
6	H	16	ASP
6	H	24	CYS
6	H	33	GLN
6	H	38	LEU
6	H	39	THR
6	H	46	LEU
6	H	55	LEU
6	H	77	ARG
6	H	89	LEU
6	H	94	ASP
6	H	102	TYR
6	H	110	ASP
6	H	111	LEU
6	H	114	VAL
6	H	121	LEU
6	H	132	LEU
6	H	135	LEU
6	H	142	LEU
7	I	7	CYS
7	I	11	ASN
7	I	12	ASN
7	I	14	LEU
7	I	19	ASP
7	I	20	LYS
7	I	22	ASN

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Mol	Chain	Res	Type
7	I	24	ARG
7	I	26	LEU
7	I	29	CYS
7	I	30	ARG
7	I	52	ILE
7	I	61	ASP
7	I	62	ILE
7	I	64	SER
7	I	79	HIS
7	I	83	ASN
7	I	91	ARG
7	I	94	ASP
7	I	95	THR
7	I	98	VAL
7	I	104	LEU
7	I	106	CYS
7	I	107	SER
8	J	1	MET
8	J	2	ILE
8	J	3	VAL
8	J	7	CYS
8	J	10	CYS
8	J	14	VAL
8	J	24	LEU
8	J	28	ASP
8	J	29	GLU
8	J	43	ARG
8	J	48	ARG
9	K	5	ASP
9	K	18	LYS
9	K	20	LYS
9	K	26	LYS
9	K	32	VAL
9	K	42	LEU
9	K	47	ARG
9	K	51	LEU
9	K	55	LYS
9	K	64	GLU
9	K	67	PHE
9	K	75	ILE
9	K	78	THR
9	K	101	LEU

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Mol	Chain	Res	Type
9	K	113	THR
9	K	114	LEU
10	L	30	ILE
10	L	44	ASP
10	L	48	CYS
10	L	50	ASP
10	L	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	64	ASN
1	A	68	GLN
1	A	80	HIS
1	A	83	HIS
1	A	92	HIS
1	A	124	GLN
1	A	225	ASN
1	A	316	GLN
1	A	435	HIS
1	A	493	GLN
1	A	545	GLN
1	A	576	GLN
1	A	584	ASN
1	A	631	HIS
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	767	GLN
1	A	858	ASN
1	A	926	GLN
1	A	968	GLN
1	A	994	GLN
1	A	1033	GLN
1	A	1171	GLN
1	A	1173	HIS
1	A	1218	GLN
1	A	1232	ASN
1	A	1258	HIS
1	A	1364	ASN
1	A	1378	GLN

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Mol	Chain	Res	Type
1	A	1393	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	110	HIS
2	B	121	ASN
2	B	215	GLN
2	B	300	HIS
2	B	366	GLN
2	B	383	ASN
2	B	395	GLN
2	B	433	GLN
2	B	484	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	648	HIS
2	B	657	HIS
2	B	706	GLN
2	B	734	HIS
2	B	744	HIS
2	B	761	HIS
2	B	763	GLN
2	B	770	GLN
2	B	822	ASN
2	B	835	GLN
2	B	842	ASN
2	B	862	GLN
2	B	946	ASN
2	B	951	GLN
2	B	957	ASN
2	B	1015	HIS
2	B	1065	GLN
2	B	1074	ASN
2	B	1093	GLN
2	B	1104	HIS
2	B	1112	GLN
2	B	1177	HIS
2	B	1178	ASN
2	B	1187	ASN
2	B	1193	GLN
2	B	1195	HIS
3	C	54	ASN

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Mol	Chain	Res	Type
3	C	65	HIS
3	C	73	GLN
3	C	123	ASN
3	C	131	HIS
3	C	151	GLN
3	C	167	HIS
3	C	231	ASN
4	E	5	ASN
4	E	8	ASN
4	E	32	GLN
4	E	54	GLN
4	E	61	GLN
4	E	99	HIS
4	E	104	ASN
4	E	146	HIS
4	E	147	HIS
4	E	179	GLN
5	F	104	ASN
6	H	33	GLN
6	H	43	ASN
6	H	52	GLN
6	H	131	ASN
6	H	139	ASN
7	I	22	ASN
7	I	60	GLN
7	I	83	ASN
8	J	53	HIS
8	J	64	ASN
9	K	40	HIS
9	K	110	ASN
10	L	53	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	10/12 (83%)	6 (60%)	0

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	3	C

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Mol	Chain	Res	Type
11	R	5	A
11	R	8	G
11	R	9	G
11	R	10	A
11	R	11	G

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1395/1733 (80%)	0.09	19 (1%) 73 51	61, 90, 153, 177	0
2	B	1106/1224 (90%)	0.17	27 (2%) 59 41	57, 85, 129, 160	0
3	C	266/318 (83%)	-0.06	1 (0%) 88 74	67, 83, 112, 124	0
4	E	214/215 (99%)	0.16	6 (2%) 55 38	75, 119, 155, 165	0
5	F	84/155 (54%)	-0.02	1 (1%) 76 54	72, 95, 115, 119	0
6	H	133/146 (91%)	0.32	5 (3%) 44 31	96, 109, 138, 142	0
7	I	119/122 (97%)	0.34	4 (3%) 48 33	75, 99, 121, 136	0
8	J	65/70 (92%)	-0.13	0 100 100	66, 79, 99, 106	0
9	K	114/120 (95%)	-0.20	1 (0%) 81 60	71, 87, 98, 100	0
10	L	46/70 (65%)	0.67	5 (10%) 10 14	93, 144, 156, 157	0
11	R	11/12 (91%)	1.21	2 (18%) 3 6	65, 94, 118, 135	0
12	T	12/29 (41%)	1.23	2 (16%) 4 7	73, 91, 126, 135	0
All	All	3565/4214 (84%)	0.12	73 (2%) 65 44	57, 90, 146, 177	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	335	GLY	5.0
7	I	13	MET	4.2
2	B	883	LEU	4.1
2	B	1214	PRO	4.0
11	R	11	G	3.8
1	A	998	LEU	3.8
2	B	882	THR	3.6
1	A	168	GLY	3.6
4	E	118	PRO	3.5
10	L	45	ALA	3.4
2	B	1216	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
10	L	44	ASP	3.4
2	B	1222	ARG	3.3
2	B	265	SER	3.2
4	E	53	PRO	3.2
6	H	85	GLY	3.1
1	A	1081	LEU	3.1
2	B	480	SER	3.1
2	B	479	VAL	3.0
6	H	90	ALA	3.0
10	L	28	LYS	3.0
2	B	870	ILE	3.0
2	B	266	ALA	3.0
7	I	39	GLY	2.9
11	R	1	A	2.9
2	B	709	ASP	2.9
2	B	446	LEU	2.8
4	E	110	PHE	2.8
12	T	17	DC	2.8
1	A	1002	GLY	2.7
2	B	39	ARG	2.7
9	K	114	LEU	2.7
4	E	90	VAL	2.7
2	B	1169	MET	2.7
1	A	76	GLU	2.6
2	B	328	GLU	2.6
3	C	51	VAL	2.6
2	B	876	LYS	2.5
4	E	20	LYS	2.5
6	H	134	ASN	2.4
2	B	1103	ILE	2.4
1	A	149	GLU	2.4
2	B	937	ALA	2.4
7	I	4	PHE	2.4
6	H	130	ARG	2.4
2	B	260	GLY	2.4
1	A	75	ASN	2.3
2	B	643	ASP	2.3
1	A	51	GLY	2.3
6	H	63	LEU	2.3
1	A	1336	MET	2.3
12	T	28	DC	2.3
2	B	452	THR	2.3

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Mol	Chain	Res	Type	RSRZ
4	E	93	MET	2.3
7	I	2	THR	2.3
10	L	43	THR	2.3
1	A	176	LYS	2.2
2	B	710	LEU	2.2
2	B	222	ILE	2.2
1	A	1078	GLN	2.2
1	A	318	SER	2.2
1	A	1424	VAL	2.2
2	B	1173	ALA	2.1
5	F	154	ASP	2.1
2	B	529	GLU	2.1
1	A	999	VAL	2.1
1	A	258	GLY	2.1
2	B	305	VAL	2.1
10	L	26	THR	2.0
1	A	997	LEU	2.0
1	A	309	ALA	2.0
1	A	96	ILE	2.0
1	A	1080	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	ZN	I	203	1/1	0.93	0.07	148,148,148,148	0
13	ZN	L	105	1/1	0.95	0.08	169,169,169,169	0
13	ZN	B	1307	1/1	0.96	0.04	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	ZN	A	1735	1/1	0.97	0.05	118,118,118,118	0
13	ZN	A	1734	1/1	0.97	0.06	128,128,128,128	0
13	ZN	J	101	1/1	0.98	0.04	187,187,187,187	0
13	ZN	C	319	1/1	0.99	0.03	83,83,83,83	0
13	ZN	I	204	1/1	0.99	0.03	107,107,107,107	0

6.5 Other polymers [i](#)

There are no such residues in this entry.