



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:38 PM UTC

PDB ID : 5X50 / pdb_00005x50
Title : RNA Polymerase II from Komagataella Pastoris (Type-2 crystal)
Authors : Ehara, H.; Umehara, T.; Sekine, S.; Yokoyama, S.
Deposited on : 2017-02-14
Resolution : 4.29 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

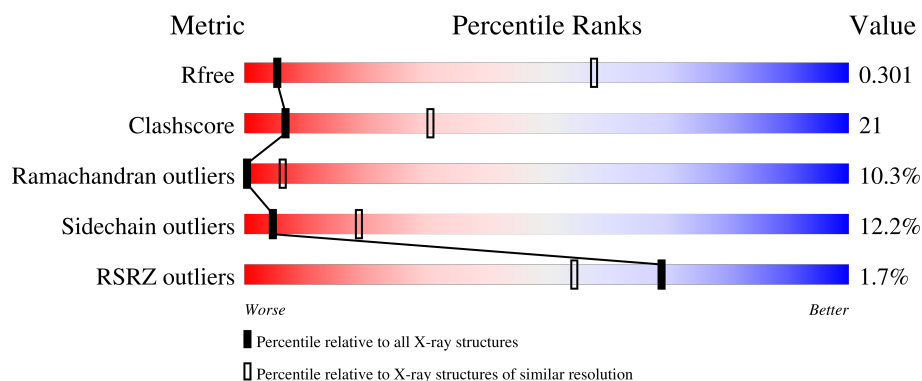
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.29 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	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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	1743	 41% 32% 8% 19%
2	B	1227	 43% 34% 10% 12%
3	C	304	 45% 34% 7% 13%
4	D	186	 41% 26% 9% 23%
5	E	214	 57% 36% 6%

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Mol	Chain	Length	Quality of chain
6	F	155	%23%26%5%46%
7	G	171	2%50%42%8%.
8	H	145	3%50%31%8%.10%
9	I	115	3%50%40%7%. .
10	J	72	%28%49%8%.11%
11	K	118	2%44%42%9%5%
12	L	73	27%26%8%.37%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28437 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 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1409	Total	C	N	O	S	0	0	0
			10410	6594	1819	1943	54			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1079	Total	C	N	O	S	0	0	0
			8241	5236	1442	1517	46			

- Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	263	Total	C	N	O	S	0	0	0
			1852	1181	308	355	8			

- Molecule 4 is a protein called RNA polymerase II subunit B32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	143	Total	C	N	O	S	0	0	0
			1004	647	170	185	2			

- Molecule 5 is a protein called RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1638	1045	288	297	8			

- Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			637	406	109	119	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1187	775	192	217	3			

- Molecule 8 is a protein called RNA polymerase subunit ABC14.5, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	131	Total	C	N	O	S	0	0	0
			965	616	155	191	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	113	Total	C	N	O	S	0	0	0
			856	537	150	158	11			

- Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	64	Total	C	N	O	S	0	0	0
			500	327	87	80	6			

- Molecule 11 is a protein called RNA polymerase II subunit B12.5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	112	Total	C	N	O	S	0	0	0
			820	535	137	146	2			

- Molecule 12 is a protein called RNA polymerase subunit, found in RNA polymerase complexes I, II, and III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			319	196	64	55	4			

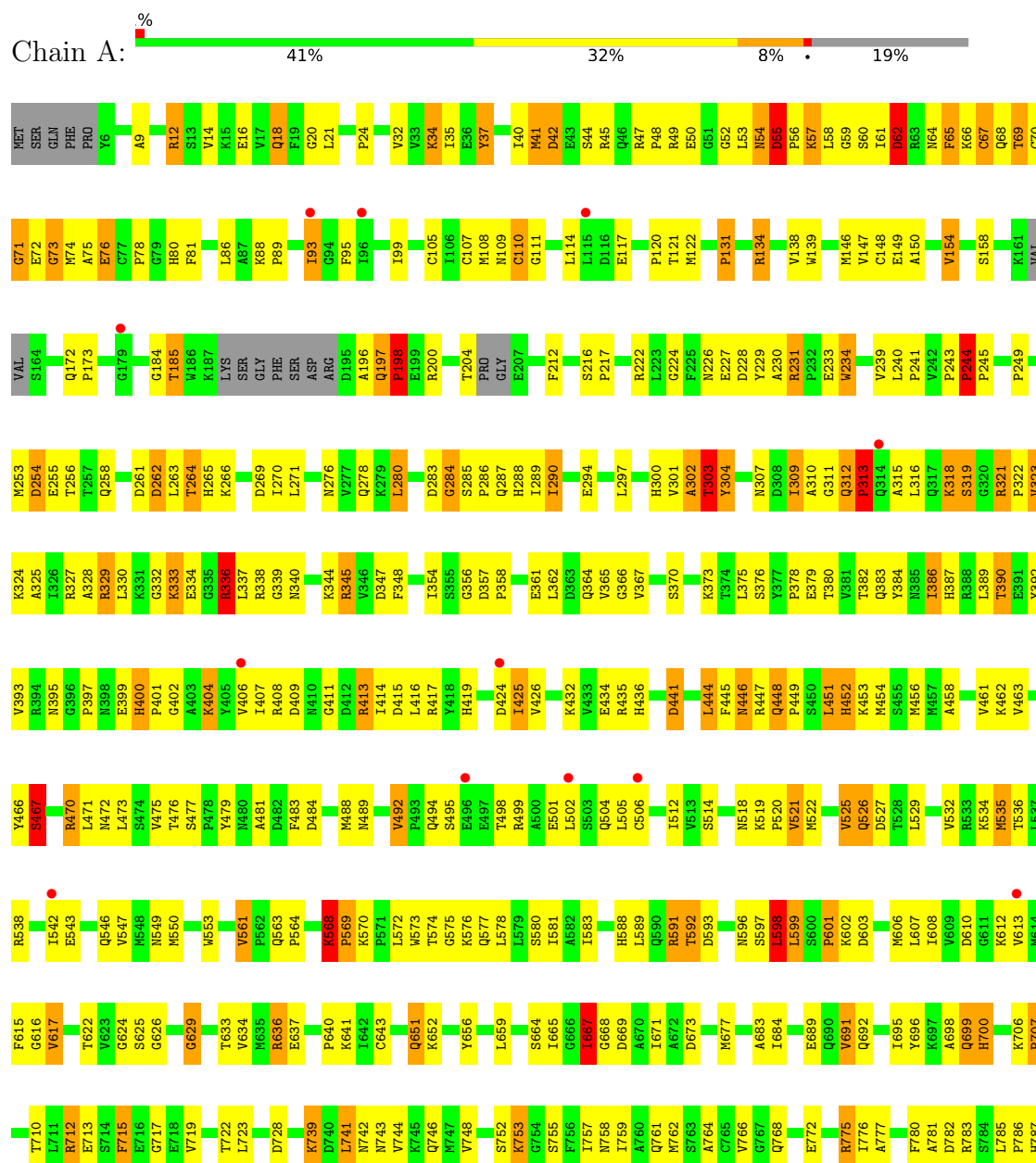
- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

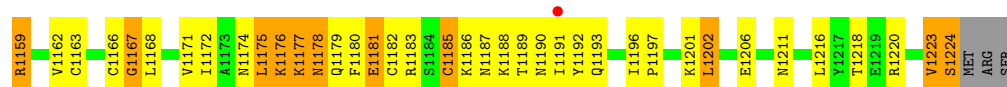
3 Residue-property plots

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.

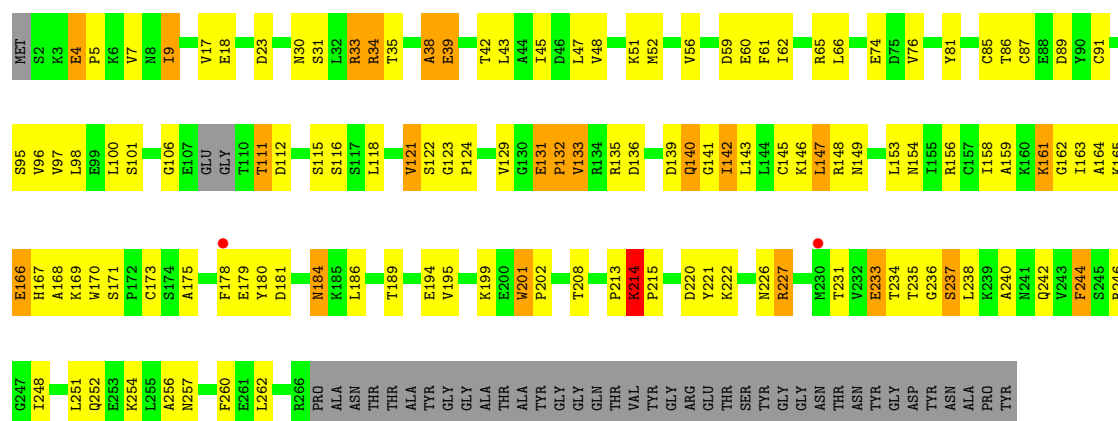
• Molecule 1: DNA-directed RNA polymerase subunit



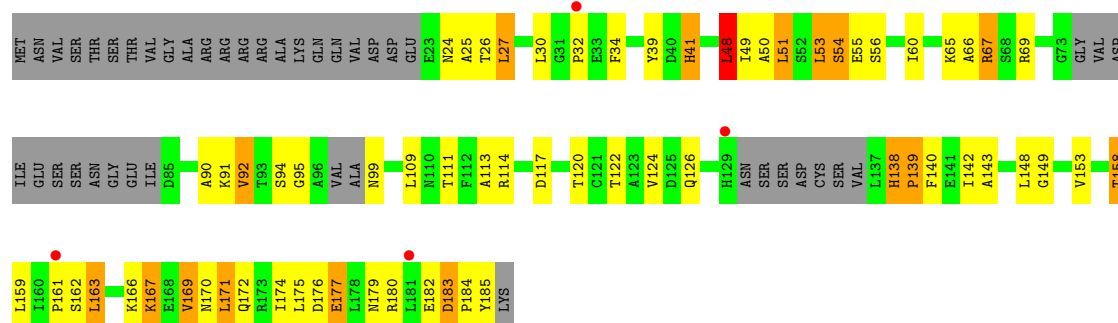
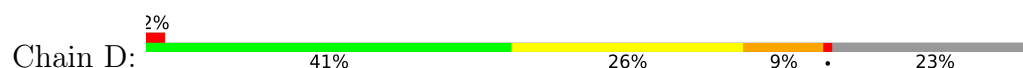
K1080	Q1084	V1085	F1086	F1087	G1088	F1089	T1090	Y1091	H996	E997	D998	R999	F1000	Y1001	Y1092	G1093	R1094	L1095	R1096	H1097	M1098	V1099	D1100	D1101	K1102	H1103	H1104	A1105	R1106	A1107	R1108	T1115	R1116	V1119	E1120	G1121	R1122	G1126	G1127	L1128	R1129	F1130	G1131	R1135	D1136	I1139	A1144	L1147	K1148	E1149	R1150	L1151	S1155	D1156	A1157	F1158
Q886	Q887	G888	T989	Y992	T993	Y994	R995	H996	E997	D998	R999	F1000	F1001	S1002	A1003	E1004	G1005	V1006	V1007	P1008	D1009	L1010	I1011	I1012	N1013	A1016	I1017	R1020	G1021	M1021	L1022	Q951	V952	L953	L954	T955	R956	N957	L961	K962	F963	V964	K965	V966	Q1065	S1066	R1067	G1068	F1069	V1071	M1072	N1073	G1075			
S844	S845	I846	D847	R848	G849	L850	F851	R852	R857	S858	Y859	H860	E863	K864	R865	S869	I870	V871	E875	K876	P877	T878	R879	A880	T881	T882	L883	R884	L885	K886	H887	G888	T889	Y890	E891	L893	D894	E895	D896	I899	A900	P901	G902	V903	S906	Q907	Q908	D909	I910	I911	I912	G913				
K914	I918	PRO	PRO	ASP	THR	GLU	GLU	LEU	GLY	GLN	ARG	THR	LYS	TYR	HIS	THR	K934	R935	D936	A937	S938	T939	P940	L941	R942	S943	T944	E945	N946	G947	I948	V949	D950	Q951	V952	L953	L954	T955	T956	L957	L961	K962	F963	V964	K965	V966	R969	T970	P974	Q975	I976	G977	F980	A981		
Q886	Q887	G888	T989	Y992	T993	Y994	R995	H996	E997	D998	R999	F1000	F1001	S1002	A1003	E1004	G1005	V1006	V1007	P1008	D1009	L1010	I1011	I1012	N1013	A1016	I1017	R1020	G1021	M1021	L1022	Q951	V952	L953	L954	T955	R956	N957	L961	K962	F963	V964	K965	V966	Q1065	S1066	R1067	G1068	F1069	V1071	M1072	N1073	G1075			
P87	T88	M89	T90	E91	A92	D93	G94	T95	T96	M99	F100	P101	Q102	E103	M108	V115	K1121	SER	MET	PHE	THR	SER	ILE	ASP	ASP	GLU	GLY	ASN	PRO	ASN	ALA	THR	LEU	ASP	TRP	GLN	GLN	VAL	HIS	GLU	PRO	ILE	LYS	ASP	GLY	VAL	GLU	GLY	ASN	K155	V156	H157	I158			
M164	L165	R166	S167	R173	T174	L175	D176	E177	V178	D179	L180	M183	K184	E185	M190	G191	G192	N197	G198	S199	E200	K201	V202	Q206	E207	R208	S209	A210	A211	N212	I213	V216	A220	A221	S222	S223	P224	I225	S226	H227	Q246	L249	Y250	G251	R252	E253	D254	K255	G256	THR						
GLY	R259	T261	T264	L265	P266	Y267	Q270	ASP	D271	L272	F273	I274	R279	G282	V283	V284	P285	D286	G287	E288	L289	Q291	Y295	D296	E297	N298	D299	V300	Q301	M302	M305	E311	F314	V315	I316	D324	F325	I326	G327	ARG	GLY	SER	ALA	ALA	LEU	GLY	ILE	ARG								
ARG	E339	R340	P341	I342	Q343	Y344	A345	R346	L347	L348	E352	P355	H356	I357	T358	G359	E360	E364	T365	R366	F369	N376	L379	L380	C381	A382	L383	E384	K385	K386	D390	H393	F394	G395	K396	R397	R398	L399	D400	L401	L405	L406	A407	N408	L409	L413	F414	R415	R416							
L417	T421	M425	C428	I429	E430	THR	ASP	ARG	ASP	PHE	ASN	LEU	ASN	L439	A440	K442	S443	T444	T445	I446	Y452	S453	G457	N458	R459	G460	Q462	E461	K463	K464	A465	M466	S467	R468	V472	S473	Q474	V475	L476	N477	R478	Y481	T484	L485	S486	H487	L488	R489	R490							
T491	N492	P493	I495	GLY	ARG	ASP	GLY	LEU	A502	K503	P504	Q506	N509	T510	G513	L514	V515	C516	E519	T520	E522	Q524	G457	N458	R459	G460	Q462	E461	K463	K464	A465	M466	S467	R468	V472	S473	Q474	V475	L476	N477	R478	Y481	T484	L485	S486	H487	L488	R489	R490							
D563	P564	T568	R572	I573	F574	V575	W579	T580	G581	I582	H583	R584	S587	M588	L589	R594	D595	L596	R597	R598	S599	G600	A601	I602	S603	E604	E605	V606	S607	I608	I609	I612	R613	E614	R615	K618	I619	F620	T621	D622	G624	R625	V626	Y627	R628	W629	G630	F631	I632	E634						
D635	D636	E637	D640	N641	LYS	GLY	E644	L645	T648	H651	T655	GLN	GLN	TYR	ASP	ASP	ALA	MET	ASN	ASP	ASP	SER	GLU	GLU	GLN	GLN	GLU	GLU	GLN	GLN	V675	V676	G677	W678	S679	T683	G685	V686	I687	E688	E695	E696	T697	L698	M699	I700	A701	M702	T703	P704	E705	D706				
L707	Q708	THR	SER	LEU	GLU	GLN	LYS	ILE	ASP	L719	N720	D721	T722	K723	A725	I726	K727	F728	GLU	MET	SER	THR	SER	SER	HIS	HIS	T737	F738	T739	H740	C741	H744	G777	W778	I747	I748	A752	S753	S754	I755	I756	P759	D760	H761	N762	Q763	S764	P765	R766	S771	A772	M773				
G774	K775	A777	L782	Y785	N786	V787	R788	M789	D790	T791	M792	T793	K794	L795	Y797	Y798	P799	Q800	K801	P802	K805	T806	Q807	A808	M809	E810	Y811	L812	K813	F814	R815	Q821	N822	A823	I824	V825	A828	C829	Y830	S831	G832	Y833	N834	Q835	E836	D837	P765	R766	S839	I840	M841	N842	Q843			
S844	S845	I846	D847	R848	G849	L850	F851	R852	R857	S858	Y859	H860	E863	K864	R865	S869	I870	V871	E875	K876	P877	T878	R879	A880	T881	T882	L883	R884	L885	K886	H887	G888	T889	Y890	E891	L893	D894	E895	D896	I899	A900	P901	G902	V903	S906	Q907	Q908	D909	I910	I911	I912	G913				
K914	I918	PRO	PRO	ASP	THR	GLU	GLU	LEU	GLY	GLN	ARG	THR	LYS	TYR	HIS	THR	K934	R935	D936	A937	S938	T939	P940	L941	R942	S943	T944	E945	N946	G947	I948	V949	D950	Q951	V952	L953	L954	T955	T956	L957	L961	K962	F963	V964	K965	V966	R969	T970	P974	Q975	I976	G977	F980	A981		
Q886	Q887	G888	T989	Y992	T993	Y994	R995	H996	E997	D998	R999	F1000	F1001	S1002	A1003	E1004	G1005	V1006	V1007	P1008	D1009	L1010	I1011	I1012	N1013	A1016	I1017	R1020	G1021	M1021	L1022	Q951	V952	L953	L954	T955	R956	N957	L961	K962	F963	V964	K965	V966	Q1065	S1066	R1067	G1068	F1069	V1071	M1072	N1073	G1075			



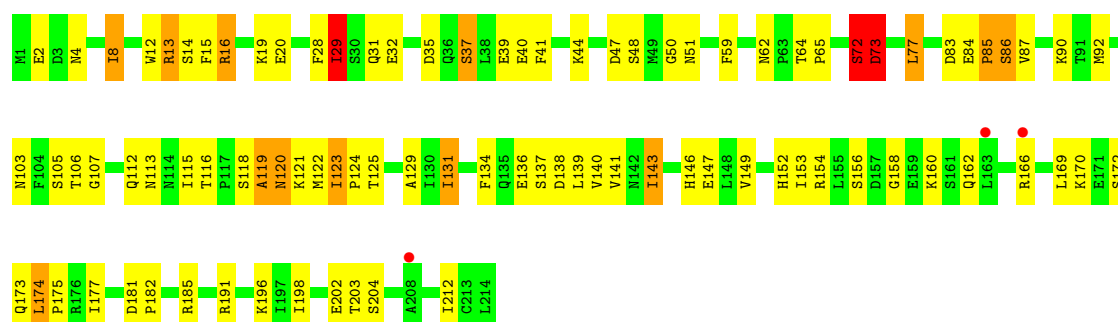
- Molecule 3: RNA polymerase II third largest subunit B44, part of central core



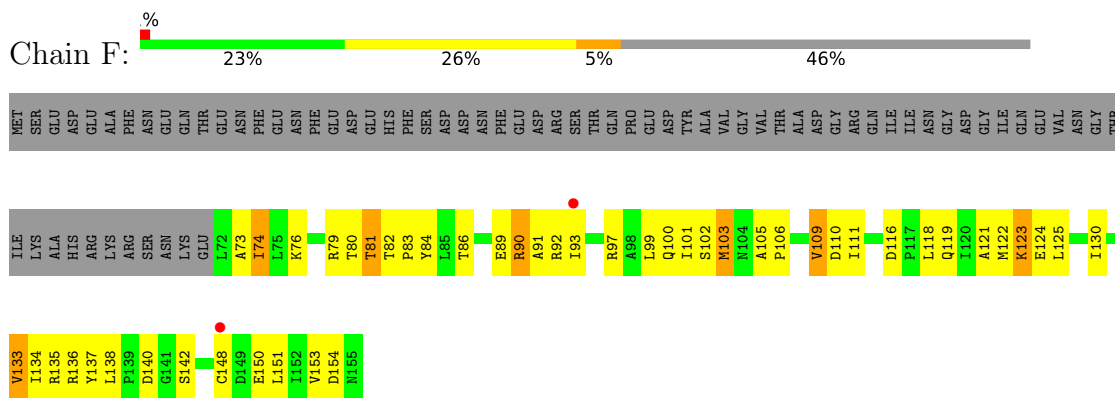
- Molecule 4: RNA polymerase II subunit B32



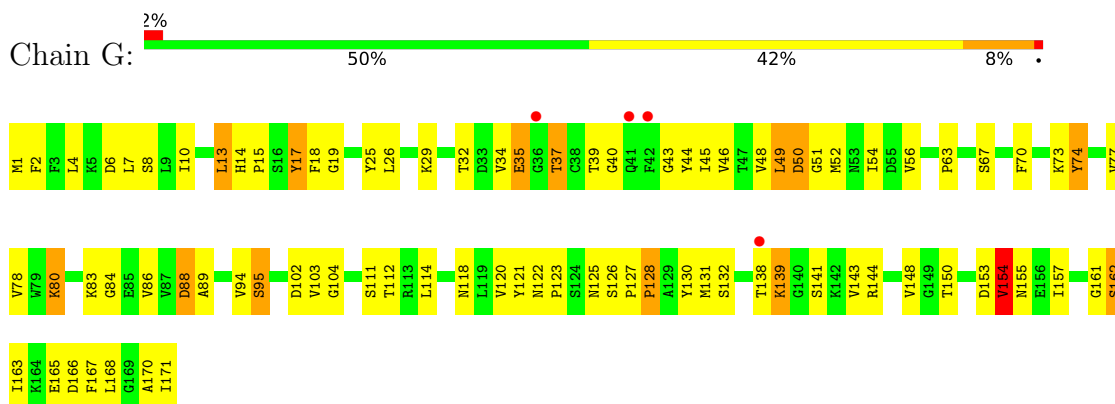
- Molecule 5: RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III



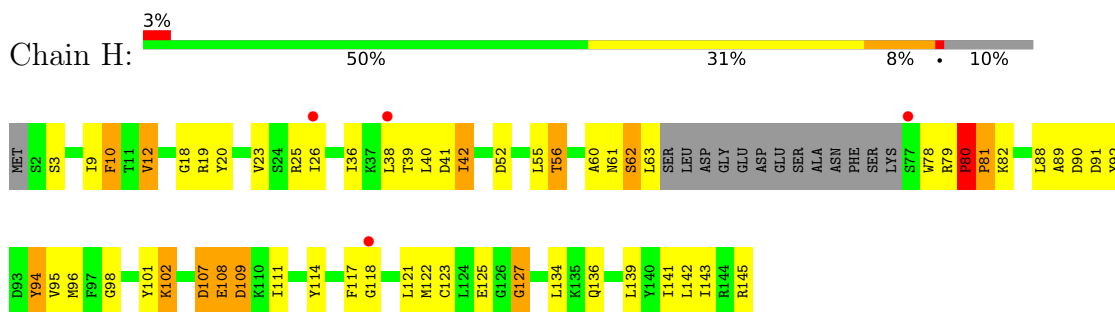
- Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III



- Molecule 7: RNA polymerase II subunit



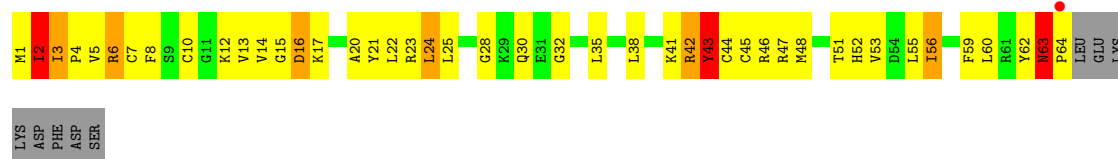
- Molecule 8: RNA polymerase subunit ABC14.5, common to RNA polymerases I, II, and III



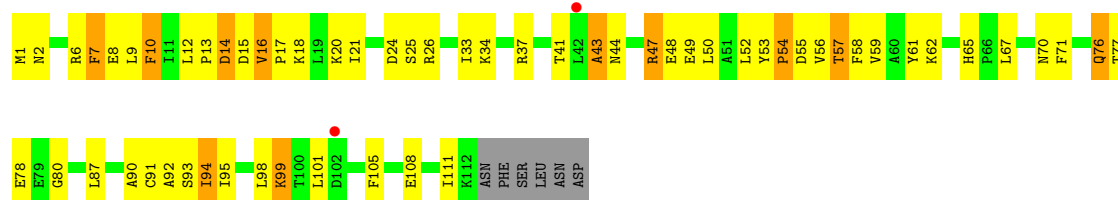
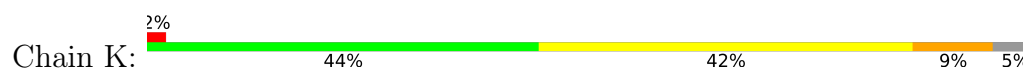
- Molecule 9: DNA-directed RNA polymerase subunit



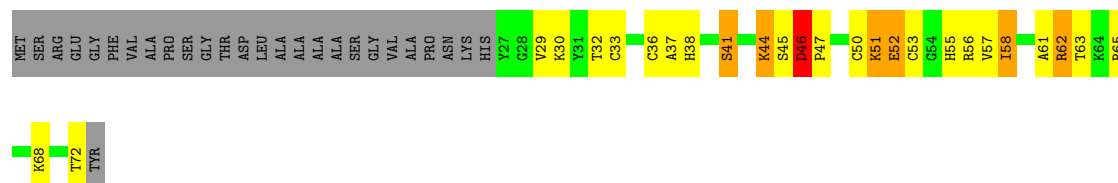
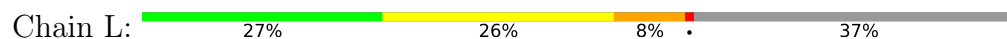
- Molecule 10: RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III



- Molecule 11: RNA polymerase II subunit B12.5



- Molecule 12: RNA polymerase subunit, found in RNA polymerase complexes I, II, and III



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	211.75Å 211.75Å 132.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.70 – 4.29 40.70 – 4.29	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.70-4.29) 99.5 (40.70-4.29)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 4.29Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.235 , 0.296 0.237 , 0.301	Depositor DCC
R_{free} test set	1992 reflections (4.40%)	wwPDB-VP
Wilson B-factor (Å ²)	191.6	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 195.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.124 for -h,-k,l 0.128 for h,-h-k,-l 0.125 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	28437	wwPDB-VP
Average B, all atoms (Å ²)	223.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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	0.42	1/10569 (0.0%)	1.19	94/14276 (0.7%)
2	B	0.40	0/8386	1.08	41/11301 (0.4%)
3	C	0.44	0/1877	1.28	21/2543 (0.8%)
4	D	0.39	0/1010	1.30	10/1357 (0.7%)
5	E	0.39	0/1668	1.05	11/2245 (0.5%)
6	F	0.39	0/646	1.16	6/873 (0.7%)
7	G	0.40	0/1207	1.14	9/1629 (0.6%)
8	H	0.41	1/980 (0.1%)	0.98	1/1324 (0.1%)
9	I	0.40	0/871	1.06	4/1175 (0.3%)
10	J	0.48	0/509	1.16	2/684 (0.3%)
11	K	0.37	0/836	1.08	5/1131 (0.4%)
12	L	0.45	0/321	1.23	2/425 (0.5%)
All	All	0.41	2/28880 (0.0%)	1.15	206/38963 (0.5%)

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
10	J	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	887	ILE	CA-CB	7.80	1.58	1.54
8	H	80	PRO	CA-C	5.16	1.56	1.52

All (206) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	123	GLY	CA-C-N	15.15	134.67	119.82
3	C	123	GLY	C-N-CA	15.15	134.67	119.82
1	A	1279	ILE	CA-C-N	14.68	134.87	119.89
1	A	1279	ILE	C-N-CA	14.68	134.87	119.89
4	D	183	ASP	CA-C-N	14.42	134.31	120.03
4	D	183	ASP	C-N-CA	14.42	134.31	120.03
1	A	47	ARG	CA-C-N	13.15	136.28	119.84
1	A	47	ARG	C-N-CA	13.15	136.28	119.84
1	A	568	LYS	CA-C-N	-11.72	105.19	119.84
1	A	568	LYS	C-N-CA	-11.72	105.19	119.84
2	B	603	SER	CA-C-N	9.72	129.35	119.82
2	B	603	SER	C-N-CA	9.72	129.35	119.82
2	B	288	GLU	N-CA-C	-9.62	101.67	113.50
5	E	8	ILE	N-CA-C	-9.60	103.30	111.56
3	C	214	LYS	CA-C-N	9.34	131.51	119.84
3	C	214	LYS	C-N-CA	9.34	131.51	119.84
1	A	37	TYR	CA-C-N	9.12	131.93	120.89
1	A	37	TYR	C-N-CA	9.12	131.93	120.89
3	C	4	GLU	CA-C-N	-9.06	110.45	119.78
3	C	4	GLU	C-N-CA	-9.06	110.45	119.78
1	A	835	THR	N-CA-C	-8.71	101.87	111.36
1	A	1078	ALA	N-CA-C	-8.52	103.47	114.04
4	D	138	HIS	CA-C-N	8.49	130.45	119.84
4	D	138	HIS	C-N-CA	8.49	130.45	119.84
4	D	176	ASP	N-CA-C	-8.21	101.92	111.03
8	H	102	LYS	N-CA-C	8.15	122.55	110.48
1	A	88	LYS	CA-C-N	8.12	128.18	119.90
1	A	88	LYS	C-N-CA	8.12	128.18	119.90
12	L	46	ASP	CA-C-N	7.71	129.47	119.84
12	L	46	ASP	C-N-CA	7.71	129.47	119.84
1	A	706	LYS	CA-C-N	7.64	129.39	119.84
1	A	706	LYS	C-N-CA	7.64	129.39	119.84
1	A	321	ARG	CA-C-N	7.54	127.42	119.05
1	A	321	ARG	C-N-CA	7.54	127.42	119.05
2	B	461	GLU	CB-CA-C	-7.47	107.95	116.54
2	B	1045	THR	CA-C-N	7.37	129.06	119.84
2	B	1045	THR	C-N-CA	7.37	129.06	119.84
2	B	633	VAL	N-CA-C	7.36	118.30	111.45
2	B	493	THR	CA-C-N	7.31	127.36	119.90
2	B	493	THR	C-N-CA	7.31	127.36	119.90
1	A	243	PRO	CA-C-N	7.29	127.88	120.38
1	A	243	PRO	C-N-CA	7.29	127.88	120.38
1	A	9	ALA	CA-C-N	7.17	127.15	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ALA	C-N-CA	7.17	127.15	119.76
1	A	302	ALA	N-CA-C	-7.14	103.42	111.14
4	D	27	LEU	N-CA-C	-7.14	104.93	112.93
1	A	1455	SER	N-CA-C	-7.11	104.58	113.18
1	A	695	ILE	N-CA-C	-6.98	104.19	111.58
6	F	103	MET	N-CA-C	-6.94	104.80	112.72
1	A	453	LYS	N-CA-C	-6.90	103.82	111.82
2	B	678	TRP	N-CA-C	-6.87	105.05	113.50
4	D	153	VAL	N-CA-C	-6.86	103.52	111.00
1	A	683	ALA	N-CA-C	-6.84	104.83	113.72
3	C	140	GLN	N-CA-C	6.83	118.46	110.41
1	A	55	ASP	CA-C-N	-6.79	111.35	119.84
1	A	55	ASP	C-N-CA	-6.79	111.35	119.84
2	B	548	ILE	N-CA-C	-6.77	104.17	110.53
9	I	65	ASP	CA-C-N	6.74	128.26	119.84
9	I	65	ASP	C-N-CA	6.74	128.26	119.84
1	A	289	ILE	N-CA-C	-6.71	106.59	113.10
2	B	1020	ARG	N-CA-C	-6.70	104.04	111.82
7	G	95	SER	CA-C-N	6.70	126.33	119.56
7	G	95	SER	C-N-CA	6.70	126.33	119.56
5	E	62	ASN	CA-C-N	6.64	128.14	119.84
5	E	62	ASN	C-N-CA	6.64	128.14	119.84
1	A	985	ILE	CA-C-N	6.58	126.02	118.85
1	A	985	ILE	C-N-CA	6.58	126.02	118.85
1	A	837	TYR	N-CA-C	-6.57	103.74	111.03
1	A	684	ILE	N-CA-C	-6.52	106.44	112.96
6	F	80	THR	N-CA-C	6.50	121.25	113.12
5	E	64	THR	CA-C-N	6.49	127.00	119.47
5	E	64	THR	C-N-CA	6.49	127.00	119.47
2	B	1013	ASN	N-CA-C	6.48	117.82	109.65
1	A	1314	ILE	N-CA-C	6.46	118.35	107.18
1	A	887	ILE	CA-C-N	-6.44	113.64	120.66
1	A	887	ILE	C-N-CA	-6.44	113.64	120.66
3	C	131	GLU	CA-C-N	6.39	127.82	119.84
3	C	131	GLU	C-N-CA	6.39	127.82	119.84
1	A	1083	LEU	N-CA-C	-6.35	104.63	112.38
9	I	68	LEU	CA-C-N	6.34	126.30	120.03
9	I	68	LEU	C-N-CA	6.34	126.30	120.03
2	B	556	MET	N-CA-C	6.32	119.86	107.98
3	C	61	PHE	N-CA-C	-6.30	103.94	111.69
1	A	1136	ILE	N-CA-C	-6.28	106.41	111.81
5	E	123	ILE	CA-C-N	-6.27	112.00	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	123	ILE	C-N-CA	-6.27	112.00	119.84
1	A	280	LEU	N-CA-C	-6.23	105.35	114.39
1	A	198	PRO	CA-C-N	-6.18	113.47	122.19
1	A	198	PRO	C-N-CA	-6.18	113.47	122.19
7	G	19	GLY	CA-C-N	6.17	127.55	119.84
7	G	19	GLY	C-N-CA	6.17	127.55	119.84
1	A	492	VAL	CA-C-N	6.13	127.51	119.84
1	A	492	VAL	C-N-CA	6.13	127.51	119.84
1	A	1380	SER	N-CA-C	6.12	121.47	111.37
2	B	1009	ASP	N-CA-C	-6.11	105.95	113.41
1	A	1294	VAL	CA-C-N	6.09	127.46	119.84
1	A	1294	VAL	C-N-CA	6.09	127.46	119.84
3	C	201	TRP	CA-C-N	6.09	126.45	119.93
3	C	201	TRP	C-N-CA	6.09	126.45	119.93
1	A	290	ILE	N-CA-C	-6.06	105.81	111.45
3	C	18	GLU	N-CA-C	-6.06	101.96	110.50
2	B	651	HIS	N-CA-C	-6.03	104.79	111.36
5	E	4	ASN	N-CA-C	-6.03	105.74	114.12
1	A	1244	VAL	CA-C-N	6.00	132.51	121.70
1	A	1244	VAL	C-N-CA	6.00	132.51	121.70
1	A	244	PRO	N-CA-C	5.99	118.01	110.70
1	A	691	VAL	N-CA-C	-5.99	106.41	111.56
11	K	16	VAL	CA-C-N	-5.98	112.17	120.25
11	K	16	VAL	C-N-CA	-5.98	112.17	120.25
1	A	984	THR	N-CA-C	-5.95	102.52	110.55
2	B	1185	CYS	N-CA-C	-5.94	104.50	113.89
1	A	1265	ARG	N-CA-C	-5.93	104.76	112.23
2	B	527	GLY	N-CA-C	-5.88	106.41	114.64
2	B	86	ARG	CA-C-N	5.85	127.15	119.84
2	B	86	ARG	C-N-CA	5.85	127.15	119.84
1	A	1037	PHE	N-CA-C	5.83	118.23	107.73
2	B	291	GLN	N-CA-C	-5.83	104.83	111.07
1	A	425	ILE	N-CA-C	5.83	121.46	109.34
1	A	854	ASP	N-CA-C	-5.83	106.14	113.72
4	D	34	PHE	N-CA-C	5.81	117.41	110.44
1	A	712	ARG	N-CA-C	-5.79	104.89	111.14
2	B	599	SER	N-CA-C	-5.77	106.07	113.23
5	E	13	ARG	N-CA-C	-5.75	105.09	111.36
1	A	1191	SER	CA-C-N	5.75	126.83	120.45
1	A	1191	SER	C-N-CA	5.75	126.83	120.45
2	B	464	LYS	N-CA-C	-5.75	105.38	113.20
1	A	1328	SER	N-CA-C	-5.75	104.81	113.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	696	TYR	N-CA-C	-5.74	104.94	111.14
1	A	715	PHE	N-CA-C	-5.73	104.95	111.14
3	C	145	CYS	N-CA-C	5.73	116.85	108.14
1	A	197	GLN	CA-C-N	5.72	127.00	119.84
1	A	197	GLN	C-N-CA	5.72	127.00	119.84
3	C	38	ALA	N-CA-C	5.70	121.11	114.04
3	C	135	ARG	N-CA-C	-5.69	104.90	113.89
3	C	220	ASP	N-CA-C	-5.69	101.42	109.96
7	G	104	GLY	CA-C-N	5.68	126.63	120.83
7	G	104	GLY	C-N-CA	5.68	126.63	120.83
1	A	134	ARG	N-CA-C	-5.67	104.73	111.03
1	A	698	ALA	N-CA-C	-5.67	106.91	113.88
1	A	231	ARG	CA-C-N	5.65	126.91	119.84
1	A	231	ARG	C-N-CA	5.65	126.91	119.84
2	B	516	CYS	CA-C-N	5.64	125.17	119.19
2	B	516	CYS	C-N-CA	5.64	125.17	119.19
1	A	294	GLU	N-CA-C	-5.63	104.53	111.40
3	C	121	VAL	N-CA-C	5.63	118.93	111.17
1	A	62	ASP	N-CA-C	5.60	122.73	110.80
2	B	520	THR	CA-C-N	5.59	125.60	119.90
2	B	520	THR	C-N-CA	5.59	125.60	119.90
6	F	123	LYS	N-CA-C	-5.58	104.83	111.03
1	A	699	GLN	N-CA-C	-5.58	103.78	111.81
11	K	92	ALA	N-CA-C	-5.54	105.15	111.14
2	B	461	GLU	N-CA-C	5.53	116.71	108.31
1	A	1341	VAL	N-CA-C	5.51	116.91	111.67
6	F	148	CYS	N-CA-C	-5.51	105.82	112.54
1	A	1359	ILE	CB-CA-C	-5.46	104.88	112.04
2	B	416	LYS	N-CA-C	-5.46	106.11	112.89
2	B	528	LEU	N-CA-C	-5.46	106.30	113.17
6	F	130	ILE	CB-CA-C	-5.44	105.91	111.08
1	A	1415	ALA	N-CA-C	-5.44	107.19	113.88
3	C	254	LYS	N-CA-C	-5.43	105.01	111.03
2	B	417	LEU	N-CA-C	-5.42	105.02	111.69
1	A	1076	GLU	CA-C-N	-5.39	113.10	119.84
1	A	1076	GLU	C-N-CA	-5.39	113.10	119.84
5	E	51	ASN	CA-C-N	5.39	126.22	120.13
5	E	51	ASN	C-N-CA	5.39	126.22	120.13
11	K	52	LEU	N-CA-C	-5.39	106.38	113.12
2	B	720	ASN	N-CA-C	5.37	117.46	110.53
1	A	939	SER	N-CA-C	-5.37	105.43	111.28
1	A	1157	ASP	CA-C-N	5.36	126.21	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1157	ASP	C-N-CA	5.36	126.21	120.47
1	A	81	PHE	N-CA-C	5.36	118.05	110.50
2	B	836	GLU	N-CA-C	5.35	118.77	111.39
1	A	413	ARG	N-CA-C	5.35	117.62	108.90
4	D	67	ARG	N-CA-C	-5.33	104.36	112.04
10	J	3	ILE	CA-C-N	5.33	127.71	120.79
10	J	3	ILE	C-N-CA	5.33	127.71	120.79
11	K	99	LYS	N-CA-C	-5.33	105.37	111.07
1	A	150	ALA	N-CA-C	-5.32	106.83	113.38
2	B	466	MET	N-CA-C	-5.32	106.79	113.28
1	A	591	ARG	O-C-N	5.30	124.75	120.83
1	A	230	ALA	N-CA-C	5.28	116.17	107.20
7	G	162	SER	N-CA-C	5.27	117.20	109.24
6	F	119	GLN	N-CA-C	-5.26	104.98	111.40
2	B	805	LYS	N-CA-C	5.22	116.92	109.14
1	A	993	ARG	N-CA-C	-5.21	105.28	111.69
3	C	244	PHE	N-CA-C	-5.20	106.88	113.43
2	B	621	THR	N-CA-C	-5.19	107.49	113.88
1	A	407	ILE	N-CA-C	5.17	115.50	107.28
1	A	1066	VAL	N-CA-C	5.16	115.78	110.36
7	G	132	SER	N-CA-C	-5.15	101.93	109.81
1	A	325	ALA	N-CA-C	-5.13	102.89	110.48
2	B	1088	GLY	CA-C-N	5.12	126.24	119.84
2	B	1088	GLY	C-N-CA	5.12	126.24	119.84
2	B	596	LEU	N-CA-C	-5.12	105.78	111.36
1	A	367	VAL	CA-C-N	5.10	125.39	119.93
1	A	367	VAL	C-N-CA	5.10	125.39	119.93
1	A	583	ILE	CA-C-N	5.08	125.02	119.78
1	A	583	ILE	C-N-CA	5.08	125.02	119.78
2	B	881	THR	N-CA-C	5.08	121.61	110.80
4	D	39	TYR	N-CA-C	5.07	117.24	109.07
3	C	39	GLU	N-CA-C	5.07	118.95	112.26
2	B	549	ASN	N-CA-C	-5.06	105.45	110.97
7	G	86	VAL	N-CA-C	5.05	115.12	107.75
1	A	400	HIS	CA-C-N	-5.01	113.58	119.84
1	A	400	HIS	C-N-CA	-5.01	113.58	119.84
1	A	809	LEU	N-CA-C	5.01	121.47	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	30	GLN	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	10410	0	9856	480	0
2	B	8241	0	7943	401	0
3	C	1852	0	1639	79	0
4	D	1004	0	913	42	0
5	E	1638	0	1551	49	0
6	F	637	0	620	35	0
7	G	1187	0	1092	56	0
8	H	965	0	864	39	0
9	I	856	0	774	46	0
10	J	500	0	503	55	0
11	K	820	0	719	39	0
12	L	319	0	288	14	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
All	All	28437	0	26762	1179	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 21.

All (1179) 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:285:PRO:HB2	9:I:11:ASN:HB3	1.30	1.13
1:A:256:THR:H	2:B:935:ARG:HH12	1.10	0.97
1:A:67:CYS:SG	1:A:80:HIS:NE2	2.41	0.93
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.56	0.87
1:A:226:ASN:HD22	1:A:229:TYR:H	1.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.59	0.84
1:A:40:ILE:HB	1:A:41:MET:HE2	1.59	0.84
3:C:165:LYS:O	11:K:6:ARG:NH1	2.11	0.84
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.41	0.84
4:D:50:ALA:HB1	4:D:143:ALA:HB2	1.60	0.83
6:F:109:VAL:HG12	6:F:110:ASP:H	1.42	0.83
3:C:65:ARG:NH2	10:J:3:ILE:O	2.13	0.81
2:B:899:ILE:HG22	2:B:903:VAL:HG21	1.63	0.80
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.64	0.80
1:A:60:SER:OG	1:A:64:ASN:O	1.99	0.80
3:C:171:SER:O	10:J:6:ARG:NH2	2.14	0.79
3:C:42:THR:HG22	3:C:43:LEU:H	1.45	0.79
2:B:848:ARG:NH1	10:J:8:PHE:O	2.16	0.79
2:B:1159:ARG:HH11	2:B:1159:ARG:HB3	1.48	0.78
1:A:446:ASN:HB2	1:A:456:MET:HG2	1.66	0.78
1:A:700:HIS:HA	9:I:113:GLU:HA	1.66	0.77
2:B:799:PRO:HG2	10:J:55:LEU:HD11	1.67	0.77
11:K:56:VAL:HA	11:K:77:THR:HG22	1.67	0.77
1:A:122:MET:HE1	1:A:138:VAL:HG13	1.67	0.76
1:A:710:THR:HB	1:A:713:GLU:HG3	1.68	0.75
2:B:300:TRP:CZ3	9:I:45:ARG:HB3	2.20	0.74
1:A:780:PHE:HE1	1:A:786:PRO:HD3	1.53	0.74
2:B:270:GLN:HG2	2:B:271:ASP:H	1.52	0.73
2:B:766:ARG:HH22	2:B:1020:ARG:HH11	1.36	0.73
3:C:74:GLU:O	3:C:246:ARG:NH2	2.17	0.73
2:B:509:ASN:N	2:B:509:ASN:HD22	1.87	0.73
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.71	0.73
6:F:82:THR:HG22	6:F:84:TYR:H	1.51	0.73
2:B:202:VAL:HG21	2:B:476:LEU:HD13	1.71	0.73
2:B:800:GLN:HG2	10:J:51:THR:HG22	1.70	0.73
2:B:52:GLU:HG3	2:B:53:GLU:H	1.53	0.72
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.71	0.72
1:A:739:LYS:H	1:A:739:LYS:HD2	1.55	0.71
1:A:1241:ARG:HH22	1:A:1243:ARG:HH22	1.36	0.71
3:C:175:ALA:HB3	10:J:42:ARG:HH22	1.53	0.71
1:A:787:HIS:CD2	2:B:700:ILE:HB	2.26	0.71
1:A:913:VAL:O	1:A:981:SER:N	2.24	0.71
2:B:22:SER:HA	2:B:811:TYR:HE2	1.56	0.71
3:C:38:ALA:HA	3:C:164:ALA:HB3	1.73	0.70
2:B:225:ILE:HA	2:B:250:TYR:HA	1.73	0.70
1:A:1104:LYS:HG2	1:A:1108:ASN:HD21	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:83:ASP:O	5:E:85:PRO:HD3	1.91	0.70
1:A:447:ARG:HB2	1:A:488:MET:SD	2.31	0.70
1:A:1074:ILE:HD11	1:A:1371:MET:HA	1.73	0.70
8:H:40:LEU:HD22	8:H:122:MET:HE3	1.74	0.70
2:B:822:ASN:O	10:J:47:ARG:NH1	2.24	0.70
9:I:106:CYS:SG	9:I:107:LYS:N	2.64	0.70
1:A:333:LYS:H	1:A:338:ARG:HB3	1.57	0.70
2:B:942:ARG:HB2	2:B:945:GLU:HG3	1.73	0.70
1:A:538:ARG:HD2	8:H:20:TYR:HE1	1.56	0.69
2:B:806:THR:HG22	2:B:808:ALA:H	1.57	0.69
1:A:336:ARG:HA	1:A:340:ASN:HD22	1.57	0.69
1:A:710:THR:HG22	1:A:712:ARG:H	1.56	0.69
2:B:941:LEU:HD21	2:B:946:ASN:HA	1.74	0.69
1:A:93:ILE:HG21	1:A:302:ALA:HA	1.74	0.69
1:A:1084:ASN:HB3	1:A:1086:PHE:HD1	1.57	0.69
2:B:860:MET:HB2	2:B:965:LYS:HG2	1.74	0.69
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.74	0.69
10:J:1:MET:HB2	10:J:55:LEU:HD12	1.75	0.69
1:A:739:LYS:HB2	1:A:741:LEU:HD23	1.74	0.68
2:B:821:GLN:HE22	2:B:851:PHE:H	1.40	0.68
2:B:287:GLY:H	2:B:290:LEU:HD23	1.56	0.68
1:A:68:GLN:HE21	1:A:80:HIS:CE1	2.11	0.68
1:A:70:CYS:HB3	2:B:1172:ILE:HG23	1.73	0.68
1:A:780:PHE:CE1	1:A:786:PRO:HD3	2.28	0.68
2:B:503:LYS:HG2	2:B:504:PRO:HD3	1.75	0.68
3:C:233:GLU:OE1	10:J:12:LYS:HE2	1.94	0.68
9:I:34:TYR:HD2	9:I:35:THR:N	1.91	0.68
1:A:240:LEU:HD12	1:A:241:PRO:HD2	1.76	0.68
2:B:594:ARG:O	2:B:598:ARG:HG3	1.93	0.68
1:A:380:THR:HG22	1:A:432:LYS:HG2	1.76	0.68
1:A:1118:LEU:HB2	1:A:1332:SER:HA	1.76	0.68
1:A:451:LEU:HD22	1:A:1079:THR:HG21	1.76	0.67
1:A:1351:LEU:HG	1:A:1375:VAL:HG22	1.76	0.67
2:B:997:GLU:HB3	3:C:34:ARG:HB3	1.76	0.67
1:A:527:ASP:OD1	2:B:1013:ASN:ND2	2.22	0.67
1:A:636:ARG:HA	1:A:636:ARG:HH11	1.58	0.67
2:B:1181:GLU:HA	2:B:1188:LYS:HG2	1.76	0.67
1:A:781:ALA:N	2:B:696:GLU:OE1	2.24	0.67
4:D:90:ALA:O	4:D:92:VAL:N	2.25	0.67
4:D:24:ASN:O	7:G:83:LYS:HD2	1.94	0.67
2:B:1006:ILE:HG22	10:J:44:CYS:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:GLU:HB2	1:A:364:GLN:HG3	1.76	0.66
2:B:1099:VAL:O	2:B:1101:ASP:N	2.28	0.66
9:I:95:THR:HG22	9:I:96:ASN:H	1.60	0.66
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.78	0.66
4:D:53:LEU:O	4:D:55:GLU:N	2.27	0.66
12:L:36:CYS:O	12:L:38:HIS:N	2.29	0.65
2:B:514:LEU:HD22	2:B:626:VAL:HG12	1.79	0.65
3:C:142:ILE:HG22	10:J:15:GLY:HA3	1.78	0.65
2:B:882:THR:HG1	2:B:934:LYS:N	1.95	0.65
10:J:42:ARG:H	10:J:42:ARG:HD3	1.60	0.65
5:E:134:PHE:HB3	5:E:139:LEU:HD11	1.78	0.65
3:C:116:SER:HB3	3:C:140:GLN:HB3	1.77	0.65
9:I:50:THR:HG22	9:I:51:ASN:H	1.61	0.65
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.11	0.65
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.78	0.64
1:A:347:ASP:HB3	2:B:1108:ARG:H	1.63	0.64
2:B:519:GLU:HB2	2:B:752:ALA:HB3	1.80	0.64
2:B:1004:GLU:HB2	2:B:1006:ILE:HG12	1.80	0.64
3:C:147:LEU:HA	10:J:60:LEU:HD21	1.78	0.64
9:I:50:THR:OG1	9:I:92:ARG:NH1	2.30	0.64
2:B:847:ASP:HB3	3:C:167:HIS:CD2	2.33	0.64
1:A:883:THR:O	1:A:1027:ARG:NH2	2.29	0.64
3:C:65:ARG:NH1	10:J:2:ILE:HG21	2.13	0.64
5:E:47:ASP:CG	5:E:48:SER:H	2.04	0.64
2:B:33:GLN:HG3	2:B:34:GLN:H	1.63	0.64
2:B:95:THR:OG1	2:B:96:THR:N	2.28	0.64
1:A:1078:ALA:HA	1:A:1081:MET:HE2	1.80	0.64
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.78	0.64
1:A:542:ILE:HD13	1:A:550:MET:HE1	1.78	0.64
1:A:1129:ASP:HB3	1:A:1132:LYS:HB3	1.80	0.64
1:A:1326:ASP:C	1:A:1328:SER:H	2.06	0.64
7:G:138:THR:HG22	7:G:139:LYS:H	1.62	0.63
2:B:954:LEU:HA	2:B:964:VAL:HG22	1.79	0.63
5:E:116:THR:HG22	5:E:118:SER:H	1.63	0.63
1:A:256:THR:OG1	2:B:935:ARG:NH1	2.31	0.63
2:B:801:LYS:O	10:J:51:THR:HG23	1.98	0.63
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.34	0.63
1:A:783:ARG:NH2	2:B:696:GLU:O	2.31	0.63
2:B:551:LEU:C	2:B:553:GLU:H	2.06	0.63
3:C:100:LEU:HD13	3:C:118:LEU:HD23	1.81	0.63
2:B:1069:PHE:HD1	2:B:1069:PHE:H	1.43	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:95:ILE:O	11:K:99:LYS:N	2.29	0.63
1:A:1397:THR:HG22	1:A:1398:GLY:H	1.64	0.62
2:B:305:MET:HE2	2:B:383:LEU:HD21	1.81	0.62
1:A:16:GLU:HG2	1:A:1421:LEU:HD11	1.81	0.62
2:B:798:TYR:HD1	10:J:4:PRO:HG3	1.64	0.62
1:A:86:LEU:HD21	1:A:240:LEU:HB2	1.81	0.62
2:B:596:LEU:HB3	2:B:602:ILE:HD11	1.81	0.62
3:C:161:LYS:O	3:C:170:TRP:NE1	2.32	0.62
1:A:69:THR:C	1:A:71:GLY:H	2.07	0.62
2:B:341:ARG:O	2:B:345:ALA:N	2.30	0.62
2:B:885:LEU:HA	2:B:936:ASP:HB3	1.80	0.62
1:A:1447:MET:HE1	6:F:135:ARG:CB	2.30	0.62
1:A:1450:GLU:HA	1:A:1453:LEU:HB3	1.80	0.62
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.81	0.62
2:B:837:ASP:OD2	2:B:1020:ARG:NH2	2.32	0.62
1:A:529:LEU:O	1:A:532:VAL:HG12	1.99	0.62
1:A:882:GLN:NE2	1:A:960:VAL:O	2.33	0.62
1:A:880:GLU:OE1	1:A:964:ARG:NH2	2.33	0.62
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.82	0.62
2:B:1223:VAL:O	2:B:1224:SER:HB2	1.98	0.62
9:I:13:MET:HE3	9:I:14:LEU:H	1.65	0.62
1:A:41:MET:HB3	1:A:49:ARG:HA	1.81	0.62
1:A:266:LYS:H	1:A:266:LYS:HD2	1.65	0.62
6:F:86:THR:OG1	6:F:89:GLU:HG3	2.00	0.62
1:A:1116:PRO:HB2	1:A:1314:ILE:HG23	1.80	0.61
1:A:357:ASP:OD2	11:K:65:HIS:HE1	1.82	0.61
1:A:380:THR:OG1	6:F:102:SER:HB2	2.00	0.61
2:B:1033:LYS:NZ	2:B:1068:GLY:O	2.33	0.61
2:B:1166:CYS:O	2:B:1168:LEU:N	2.32	0.61
1:A:354:ILE:HG21	1:A:488:MET:HG3	1.82	0.61
2:B:556:MET:HE1	2:B:573:ILE:CG1	2.29	0.61
2:B:889:THR:HG22	2:B:891:GLU:H	1.65	0.61
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.40	0.61
2:B:41:PHE:HA	2:B:45:SER:HB2	1.81	0.61
1:A:37:TYR:HB2	1:A:52:GLY:HA3	1.82	0.61
1:A:568:LYS:HD2	1:A:569:PRO:HD2	1.83	0.61
1:A:598:LEU:O	1:A:599:LEU:HB2	2.01	0.61
1:A:891:ASP:OD1	1:A:941:ARG:NH1	2.32	0.61
5:E:174:LEU:HD23	5:E:175:PRO:HD2	1.82	0.61
3:C:30:ASN:O	3:C:33:ARG:HB3	2.00	0.60
10:J:1:MET:N	10:J:55:LEU:H	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PRO:HD2	1:A:234:TRP:CD1	2.36	0.60
1:A:512:ILE:HA	1:A:522:MET:HE3	1.82	0.60
1:A:542:ILE:HG21	1:A:550:MET:HE1	1.84	0.60
2:B:401:LEU:HD13	2:B:538:ILE:HD12	1.84	0.60
8:H:92:TYR:HB3	8:H:143:ILE:O	2.01	0.60
1:A:1373:LEU:O	1:A:1377:VAL:HG23	2.00	0.60
2:B:357:ILE:O	2:B:358:THR:HB	2.01	0.60
2:B:513:GLY:HA2	2:B:748:ILE:HG22	1.84	0.60
3:C:146:LYS:HB2	10:J:60:LEU:HD11	1.83	0.60
2:B:910:ILE:HA	2:B:940:PRO:HA	1.83	0.60
3:C:56:VAL:HG11	10:J:59:PHE:HB3	1.82	0.60
9:I:16:PRO:HB2	9:I:25:LEU:HD11	1.83	0.60
3:C:175:ALA:CB	10:J:42:ARG:HH22	2.15	0.60
4:D:41:HIS:HB2	7:G:73:LYS:HE3	1.83	0.60
2:B:559:LEU:HB2	2:B:581:GLY:HA2	1.82	0.60
1:A:266:LYS:HD2	1:A:266:LYS:N	2.17	0.60
1:A:286:PRO:O	1:A:288:HIS:N	2.35	0.60
1:A:1217:LYS:O	1:A:1221:VAL:HG23	2.02	0.60
2:B:612:ILE:C	2:B:614:GLU:H	2.10	0.60
2:B:785:TYR:HE2	10:J:59:PHE:CE1	2.20	0.60
1:A:397:PRO:HG3	1:A:417:ARG:HB3	1.83	0.60
2:B:755:ILE:HG22	2:B:809:MET:HE2	1.84	0.60
1:A:1132:LYS:O	1:A:1136:ILE:HG13	2.02	0.59
10:J:43:TYR:HA	10:J:46:ARG:HB2	1.84	0.59
8:H:88:LEU:C	8:H:90:ASP:H	2.10	0.59
2:B:981:ALA:HB3	2:B:1095:LEU:HD11	1.83	0.59
3:C:248:ILE:HG23	11:K:98:LEU:HD13	1.83	0.59
1:A:615:PHE:HB3	8:H:121:LEU:HD21	1.84	0.59
1:A:95:PHE:O	1:A:99:ILE:HG13	2.03	0.59
1:A:1326:ASP:O	1:A:1328:SER:N	2.33	0.59
3:C:34:ARG:HD3	11:K:41:THR:OG1	2.03	0.59
3:C:252:GLN:HE21	11:K:95:ILE:HG23	1.68	0.59
1:A:856:THR:HG21	1:A:858:ARG:HE	1.67	0.59
2:B:852:ARG:HH22	12:L:72:THR:HA	1.68	0.59
7:G:138:THR:HG22	7:G:139:LYS:N	2.17	0.59
2:B:597:ARG:NH2	2:B:606:VAL:O	2.35	0.59
3:C:184:ASN:HD21	3:C:189:THR:HB	1.68	0.59
5:E:146:HIS:HB3	5:E:149:VAL:HG23	1.84	0.59
9:I:71:SER:HB3	9:I:85:PHE:CE2	2.37	0.59
1:A:303:THR:HG22	1:A:304:TYR:N	2.18	0.59
1:A:1136:ILE:HG22	1:A:1140:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LEU:C	1:A:265:HIS:H	2.11	0.58
2:B:975:GLN:O	2:B:977:GLY:N	2.35	0.58
1:A:934:TYR:O	1:A:938:VAL:HG23	2.03	0.58
1:A:65:PHE:O	1:A:71:GLY:HA2	2.04	0.58
1:A:1407:GLU:HB2	1:A:1411:ILE:HG13	1.85	0.58
2:B:552:GLU:HA	2:B:556:MET:HB3	1.85	0.58
2:B:957:ASN:HD22	2:B:961:LEU:HD12	1.68	0.58
3:C:91:CYS:O	3:C:95:SER:N	2.35	0.58
1:A:1118:LEU:H	1:A:1311:THR:HG22	1.68	0.58
2:B:265:LEU:HD12	2:B:272:ILE:HD12	1.85	0.58
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.85	0.58
1:A:606:MET:HE1	1:A:613:VAL:HG13	1.85	0.58
2:B:22:SER:HA	2:B:811:TYR:CE2	2.38	0.58
3:C:31:SER:O	3:C:35:THR:HG23	2.03	0.58
3:C:115:SER:OG	3:C:141:GLY:O	2.20	0.58
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.19	0.58
10:J:42:ARG:HD3	10:J:42:ARG:N	2.19	0.58
1:A:1047:VAL:O	1:A:1051:ILE:HG13	2.04	0.58
2:B:798:TYR:CD1	10:J:4:PRO:HG3	2.38	0.58
1:A:53:LEU:HD23	1:A:54:ASN:H	1.69	0.57
1:A:870:GLY:O	5:E:203:THR:HG21	2.02	0.57
1:A:520:PRO:HG2	1:A:625:SER:HA	1.87	0.57
4:D:41:HIS:HB2	7:G:73:LYS:HZ1	1.69	0.57
1:A:309:ILE:HG22	1:A:310:ALA:H	1.69	0.57
2:B:466:MET:HE3	2:B:467:SER:HA	1.87	0.57
2:B:1129:ARG:HG2	2:B:1131:GLY:H	1.68	0.57
1:A:1199:LEU:HD11	1:A:1240:ILE:HD11	1.86	0.57
2:B:810:GLU:HA	2:B:815:ARG:HH12	1.70	0.57
1:A:484:ASP:HB2	2:B:987:LYS:HG3	1.87	0.57
2:B:594:ARG:NH2	2:B:608:ILE:O	2.38	0.57
3:C:252:GLN:O	3:C:256:ALA:N	2.37	0.57
1:A:345:ARG:HA	2:B:1129:ARG:HA	1.87	0.57
2:B:352:GLU:O	2:B:355:PRO:HD3	2.05	0.57
2:B:509:ASN:HD22	2:B:509:ASN:H	1.53	0.57
4:D:49:ILE:HG21	7:G:4:LEU:HB2	1.86	0.57
1:A:339:GLY:HA2	2:B:1129:ARG:HH22	1.69	0.57
3:C:48:VAL:O	12:L:68:LYS:HA	2.05	0.57
9:I:44:TYR:OH	9:I:46:HIS:ND1	2.30	0.57
1:A:495:SER:HB2	2:B:1149:GLU:OE2	2.05	0.56
1:A:931:ASN:O	1:A:935:GLU:N	2.30	0.56
2:B:645:LEU:HG	2:B:708:GLN:HE22	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:20:LYS:HB3	11:K:34:LYS:HB2	1.87	0.56
10:J:35:LEU:HB3	10:J:46:ARG:HH12	1.70	0.56
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.87	0.56
1:A:134:ARG:O	1:A:138:VAL:HG23	2.05	0.56
1:A:775:ARG:NH2	1:A:798:LYS:HG3	2.20	0.56
1:A:859:ASN:HD22	1:A:859:ASN:C	2.13	0.56
1:A:1014:GLN:O	1:A:1017:THR:OG1	2.23	0.56
1:A:1066:VAL:HG12	1:A:1373:LEU:HD22	1.87	0.56
1:A:1437:ALA:O	1:A:1439:MET:N	2.38	0.56
2:B:797:TYR:O	10:J:1:MET:HG2	2.05	0.56
2:B:882:THR:O	2:B:883:LEU:HB2	2.04	0.56
1:A:597:SER:O	1:A:599:LEU:N	2.38	0.56
1:A:829:ALA:HB1	2:B:523:GLY:HA2	1.88	0.56
10:J:23:ARG:C	10:J:25:LEU:H	2.14	0.56
3:C:97:VAL:N	3:C:122:SER:OG	2.36	0.56
7:G:8:SER:HB3	7:G:73:LYS:HD2	1.86	0.56
1:A:1166:GLU:O	1:A:1168:ASP:N	2.35	0.56
1:A:1166:GLU:C	1:A:1168:ASP:H	2.12	0.56
1:A:1445:ASP:HB2	6:F:137:TYR:HE1	1.70	0.56
1:A:526:GLN:OE1	2:B:836:GLU:N	2.22	0.56
2:B:384:GLU:HB3	9:I:91:ARG:O	2.05	0.56
1:A:1376:ASP:HA	1:A:1379:THR:HG22	1.88	0.56
2:B:287:GLY:HA2	9:I:6:PHE:HE1	1.71	0.56
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.39	0.56
7:G:44:TYR:HE1	7:G:157:ILE:HB	1.71	0.56
2:B:540:ILE:N	2:B:605:GLU:OE2	2.39	0.56
6:F:97:ARG:HA	6:F:100:GLN:HG3	1.86	0.56
1:A:444:LEU:HD23	1:A:502:LEU:HD21	1.88	0.56
1:A:504:GLN:HE22	6:F:90:ARG:HH21	1.54	0.55
1:A:822:ARG:HH11	1:A:822:ARG:HB2	1.70	0.55
1:A:1449:ASP:HB2	6:F:133:VAL:HG21	1.87	0.55
2:B:379:LEU:HA	2:B:382:ALA:HB3	1.87	0.55
4:D:41:HIS:HB2	7:G:73:LYS:CE	2.35	0.55
4:D:51:LEU:HB2	7:G:2:PHE:O	2.06	0.55
9:I:16:PRO:HA	9:I:27:TYR:HA	1.87	0.55
10:J:63:ASN:HB3	10:J:64:PRO:CD	2.36	0.55
1:A:316:LEU:HB2	2:B:464:LYS:HB3	1.86	0.55
2:B:286:ASP:C	2:B:288:GLU:H	2.14	0.55
2:B:648:THR:H	2:B:651:HIS:HD2	1.52	0.55
5:E:90:LYS:C	5:E:92:MET:H	2.15	0.55
8:H:88:LEU:O	8:H:90:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:10:PHE:HA	11:K:37:ARG:HB3	1.88	0.55
1:A:392:TYR:O	1:A:402:GLY:HA2	2.06	0.55
1:A:591:ARG:HD2	1:A:606:MET:HB3	1.86	0.55
1:A:817:HIS:CD2	2:B:764:SER:HB2	2.41	0.55
2:B:476:LEU:HA	2:B:487:HIS:ND1	2.21	0.55
6:F:82:THR:O	6:F:136:ARG:NH1	2.32	0.55
1:A:546:GLN:HG2	1:A:550:MET:HE2	1.88	0.55
2:B:417:LEU:HD22	2:B:446:ILE:HD11	1.89	0.55
2:B:766:ARG:NH2	2:B:1020:ARG:HH11	2.05	0.55
10:J:42:ARG:H	10:J:42:ARG:CD	2.19	0.55
1:A:454:MET:HE3	1:A:521:VAL:HG11	1.88	0.55
2:B:356:HIS:O	2:B:357:ILE:HB	2.07	0.55
9:I:7:CYS:O	9:I:11:ASN:HA	2.07	0.55
1:A:348:PHE:H	2:B:1107:ALA:HA	1.72	0.55
2:B:398:ARG:O	2:B:399:LEU:HD23	2.07	0.55
2:B:773:MET:SD	2:B:987:LYS:HD3	2.47	0.55
1:A:1156:TYR:OH	9:I:18:GLU:OE2	2.25	0.55
2:B:325:PHE:O	2:B:326:ILE:HG13	2.06	0.55
5:E:107:GLY:HA3	5:E:131:ILE:HG23	1.89	0.55
11:K:65:HIS:CD2	11:K:67:LEU:H	2.25	0.55
1:A:822:ARG:O	1:A:826:ILE:HG13	2.07	0.54
2:B:199:SER:OG	2:B:201:LYS:NZ	2.39	0.54
1:A:943:PHE:HD2	1:A:944:LEU:HD23	1.72	0.54
3:C:133:VAL:HG21	3:C:237:SER:HA	1.89	0.54
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.88	0.54
1:A:146:MET:HA	1:A:172:GLN:HE21	1.72	0.54
1:A:400:HIS:HB3	1:A:401:PRO:HD3	1.90	0.54
2:B:1096:ARG:HD2	2:B:1097:HIS:ND1	2.22	0.54
2:B:302:MET:HE2	2:B:379:LEU:HD12	1.90	0.54
2:B:995:ARG:O	2:B:999:MET:HB2	2.08	0.54
8:H:12:VAL:HB	8:H:52:ASP:H	1.73	0.54
2:B:1095:LEU:HD12	2:B:1095:LEU:H	1.71	0.54
1:A:835:THR:HG21	1:A:1079:THR:HG23	1.90	0.54
1:A:1165:ILE:HB	1:A:1168:ASP:HB2	1.89	0.54
2:B:249:LEU:HD13	2:B:261:ILE:HG12	1.90	0.54
2:B:366:ARG:HG2	2:B:559:LEU:HD23	1.90	0.54
2:B:912:ILE:O	2:B:938:SER:HB3	2.08	0.54
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.89	0.54
7:G:148:VAL:H	7:G:161:GLY:HA2	1.71	0.54
8:H:111:ILE:H	8:H:127:GLY:HA2	1.71	0.54
1:A:1232:GLU:O	1:A:1234:ASN:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:763:GLN:HG2	2:B:765:PRO:HG2	1.89	0.54
1:A:780:PHE:HE2	2:B:510:THR:HG22	1.71	0.54
1:A:843:VAL:HG11	2:B:1136:ASP:OD2	2.06	0.54
2:B:609:ILE:HB	2:B:618:LYS:HB2	1.89	0.54
2:B:1181:GLU:HG2	2:B:1188:LYS:HE2	1.90	0.54
12:L:51:LYS:O	12:L:52:GLU:HB2	2.06	0.54
1:A:53:LEU:HD23	1:A:54:ASN:N	2.23	0.54
1:A:858:ARG:HD3	1:A:862:GLY:O	2.08	0.54
1:A:1228:VAL:HG13	1:A:1242:CYS:HB3	1.90	0.54
2:B:266:PRO:HG2	2:B:352:GLU:HB3	1.90	0.54
7:G:88:ASP:OD2	7:G:88:ASP:N	2.39	0.54
1:A:249:PRO:O	1:A:261:ASP:HB2	2.08	0.54
1:A:408:ARG:HD2	1:A:414:ILE:HD11	1.90	0.54
1:A:1241:ARG:NH2	1:A:1243:ARG:HH22	2.05	0.54
2:B:1072:MET:HE3	2:B:1085:VAL:HB	1.90	0.54
3:C:9:ILE:HD11	11:K:108:GLU:HB3	1.90	0.54
12:L:30:LYS:HG3	12:L:41:SER:HB2	1.89	0.54
1:A:41:MET:HE3	1:A:42:ASP:H	1.72	0.53
1:A:452:HIS:CD2	1:A:1076:GLU:HG3	2.43	0.53
1:A:467:SER:HB3	2:B:1103:ILE:HD13	1.89	0.53
1:A:1136:ILE:O	1:A:1140:ILE:HG13	2.08	0.53
11:K:47:ARG:HH11	11:K:47:ARG:HB3	1.73	0.53
1:A:318:LYS:O	1:A:319:SER:HB3	2.07	0.53
1:A:321:ARG:HH22	1:A:324:LYS:HE3	1.73	0.53
1:A:926:LEU:HD13	1:A:985:ILE:HD12	1.90	0.53
1:A:941:ARG:O	1:A:945:ARG:HG3	2.08	0.53
1:A:1447:MET:HE1	6:F:135:ARG:HB3	1.90	0.53
2:B:540:ILE:H	2:B:605:GLU:CD	2.16	0.53
2:B:810:GLU:HG3	2:B:815:ARG:HH22	1.73	0.53
2:B:890:TYR:CZ	2:B:910:ILE:HG21	2.43	0.53
3:C:52:MET:HB2	3:C:154:ASN:HB2	1.89	0.53
1:A:564:PRO:HG3	1:A:573:TRP:CZ2	2.43	0.53
1:A:1116:PRO:O	1:A:1333:ASN:ND2	2.40	0.53
2:B:285:PRO:CB	9:I:11:ASN:HB3	2.20	0.53
2:B:405:LEU:C	2:B:407:ALA:H	2.17	0.53
7:G:153:ASP:CG	7:G:154:VAL:H	2.17	0.53
1:A:284:GLY:O	1:A:286:PRO:HD3	2.09	0.53
1:A:447:ARG:HD2	1:A:481:ALA:HB2	1.89	0.53
2:B:828:ALA:O	2:B:834:ASN:ND2	2.42	0.53
9:I:32:CYS:SG	9:I:33:ASP:N	2.80	0.53
1:A:316:LEU:HD12	2:B:464:LYS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ASN:OD1	1:A:473:LEU:N	2.42	0.53
2:B:286:ASP:O	2:B:288:GLU:N	2.41	0.53
9:I:63:GLY:HA3	9:I:104:LEU:HD11	1.89	0.53
1:A:786:PRO:HG3	2:B:695:GLU:OE2	2.09	0.53
2:B:572:ARG:NH1	2:B:615:ARG:O	2.41	0.53
2:B:609:ILE:O	2:B:618:LYS:N	2.34	0.53
1:A:857:THR:HB	1:A:866:GLN:HB2	1.91	0.53
2:B:805:LYS:HB2	2:B:809:MET:SD	2.49	0.53
4:D:51:LEU:HB3	7:G:2:PHE:HB2	1.90	0.53
4:D:66:ALA:HA	4:D:69:ARG:HD2	1.89	0.53
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.91	0.53
1:A:483:PHE:O	2:B:989:THR:HG23	2.09	0.53
1:A:1328:SER:O	5:E:147:GLU:HB2	2.08	0.53
1:A:1367:ASN:HD22	1:A:1368:TYR:N	2.06	0.53
10:J:35:LEU:HA	10:J:38:LEU:HD12	1.91	0.53
1:A:400:HIS:O	1:A:402:GLY:N	2.38	0.52
1:A:568:LYS:HB2	1:A:569:PRO:CD	2.38	0.52
2:B:598:ARG:NH1	2:B:632:ILE:HD13	2.24	0.52
2:B:1094:ARG:HH21	2:B:1098:MET:HG2	1.74	0.52
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.44	0.52
12:L:33:CYS:HB2	12:L:50:CYS:SG	2.49	0.52
1:A:761:GLN:HG2	1:A:766:VAL:O	2.09	0.52
1:A:1410:GLU:H	1:A:1410:GLU:CD	2.17	0.52
2:B:1174:ASN:O	2:B:1176:LYS:N	2.43	0.52
1:A:827:ASP:O	1:A:831:LYS:HG2	2.09	0.52
2:B:1099:VAL:C	2:B:1101:ASP:H	2.18	0.52
5:E:152:HIS:O	5:E:153:ILE:HG13	2.09	0.52
1:A:55:ASP:N	1:A:56:PRO:HD3	2.24	0.52
1:A:114:LEU:HD13	1:A:172:GLN:HE22	1.75	0.52
1:A:664:SER:OG	1:A:665:ILE:N	2.43	0.52
1:A:333:LYS:N	1:A:338:ARG:HD2	2.25	0.52
1:A:890:SER:HB3	1:A:1300:GLU:HG3	1.91	0.52
2:B:226:SER:HB2	2:B:252:ARG:HA	1.92	0.52
2:B:463:LYS:C	2:B:465:ALA:H	2.18	0.52
4:D:94:SER:HB3	4:D:99:ASN:HB3	1.90	0.52
10:J:35:LEU:CB	10:J:46:ARG:HH12	2.22	0.52
1:A:310:ALA:O	1:A:312:GLN:N	2.43	0.52
1:A:1423:ASP:O	1:A:1424:CYS:HB2	2.09	0.52
2:B:369:PHE:HB3	2:B:579:TRP:CZ3	2.45	0.52
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.43	0.52
1:A:108:MET:C	1:A:110:CYS:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:TRP:CD1	11:K:62:LYS:HB2	2.44	0.52
8:H:134:LEU:HD13	8:H:136:GLN:NE2	2.25	0.52
10:J:42:ARG:HG2	10:J:44:CYS:SG	2.49	0.52
1:A:61:ILE:HG22	1:A:62:ASP:H	1.75	0.52
1:A:534:LYS:HE3	1:A:746:GLN:HE22	1.73	0.52
2:B:279:ARG:HG2	2:B:284:VAL:HA	1.92	0.52
2:B:992:VAL:HG22	2:B:993:THR:H	1.74	0.52
2:B:1003:ALA:HA	3:C:178:PHE:O	2.10	0.52
2:B:452:TYR:CG	2:B:462:GLN:HG2	2.45	0.52
10:J:16:ASP:OD1	10:J:17:LYS:HD2	2.10	0.52
2:B:180:LEU:O	2:B:183:MET:N	2.40	0.51
1:A:333:LYS:O	1:A:334:GLU:HB2	2.09	0.51
2:B:880:ALA:O	2:B:882:THR:N	2.40	0.51
2:B:1065:GLN:N	3:C:202:PRO:HG2	2.24	0.51
3:C:112:ASP:HB3	3:C:143:LEU:HD11	1.92	0.51
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.75	0.51
1:A:1388:THR:HG23	1:A:1390:HIS:H	1.76	0.51
2:B:210:ALA:HB2	2:B:398:ARG:HG2	1.92	0.51
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.92	0.51
1:A:173:PRO:HB2	1:A:184:GLY:HA3	1.93	0.51
1:A:848:ASP:OD2	1:A:860:SER:OG	2.18	0.51
1:A:1191:SER:O	1:A:1243:ARG:HD3	2.10	0.51
3:C:244:PHE:O	3:C:248:ILE:HG13	2.10	0.51
1:A:799:GLY:HA2	1:A:816:PHE:CD1	2.45	0.51
2:B:605:GLU:O	2:B:625:ARG:NH2	2.37	0.51
3:C:62:ILE:HA	3:C:65:ARG:HG3	1.92	0.51
4:D:53:LEU:C	4:D:54:SER:HG	2.17	0.51
1:A:527:ASP:HB2	2:B:835:GLN:OE1	2.11	0.51
1:A:589:LEU:HB3	1:A:608:ILE:HB	1.93	0.51
2:B:695:GLU:O	2:B:698:ILE:HG12	2.10	0.51
7:G:13:LEU:HD21	7:G:17:TYR:HB2	1.92	0.51
1:A:489:ASN:ND2	2:B:1128:LEU:HD22	2.26	0.51
1:A:1393:ASN:HD21	1:A:1411:ILE:HD11	1.75	0.51
2:B:413:LEU:O	2:B:416:LYS:N	2.42	0.51
1:A:542:ILE:HG22	1:A:547:VAL:HG23	1.92	0.51
1:A:1450:GLU:O	1:A:1454:THR:HG23	2.11	0.51
2:B:969:ARG:NH1	3:C:60:GLU:OE1	2.44	0.51
5:E:16:ARG:O	5:E:20:GLU:HG3	2.11	0.51
1:A:339:GLY:O	2:B:1129:ARG:NH1	2.40	0.51
1:A:525:VAL:HG12	1:A:526:GLN:H	1.75	0.51
1:A:1118:LEU:N	1:A:1311:THR:HG22	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1211:MET:HG2	1:A:1233:ASP:OD1	2.11	0.51
3:C:65:ARG:NH1	10:J:2:ILE:CG2	2.73	0.51
1:A:327:ARG:HB2	1:A:1409:VAL:HG21	1.93	0.50
11:K:12:LEU:HD11	11:K:18:LYS:HE2	1.93	0.50
1:A:822:ARG:HB2	1:A:822:ARG:NH1	2.25	0.50
2:B:799:PRO:HG2	10:J:55:LEU:CD1	2.38	0.50
1:A:441:ASP:O	1:A:461:VAL:HG23	2.11	0.50
1:A:640:PRO:HG2	1:A:641:LYS:H	1.76	0.50
1:A:1353:LYS:O	1:A:1357:ASN:ND2	2.45	0.50
2:B:224:PRO:O	2:B:251:GLY:N	2.43	0.50
2:B:545:GLU:HA	2:B:548:ILE:HB	1.93	0.50
6:F:92:ARG:NH2	7:G:63:PRO:HG3	2.27	0.50
1:A:1037:PHE:O	1:A:1039:LEU:N	2.44	0.50
10:J:46:ARG:HH11	10:J:46:ARG:HG2	1.76	0.50
1:A:1215:ALA:HA	1:A:1218:ILE:HD12	1.93	0.50
2:B:224:PRO:HG2	2:B:225:ILE:HD12	1.94	0.50
7:G:138:THR:CG2	7:G:139:LYS:H	2.24	0.50
12:L:32:THR:O	12:L:58:ILE:HA	2.12	0.50
1:A:322:PRO:O	1:A:323:VAL:HB	2.11	0.50
2:B:344:TYR:O	2:B:348:ILE:HG13	2.11	0.50
4:D:120:THR:O	4:D:124:VAL:HG23	2.12	0.50
8:H:134:LEU:HD13	8:H:136:GLN:HE21	1.77	0.50
11:K:87:LEU:O	11:K:91:CYS:HB2	2.11	0.50
1:A:547:VAL:HG21	1:A:573:TRP:CE3	2.46	0.50
1:A:637:GLU:OE1	1:A:968:ASN:ND2	2.45	0.50
1:A:981:SER:OG	1:A:982:ASP:N	2.35	0.50
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.76	0.50
2:B:857:ARG:HG2	2:B:859:TYR:CE1	2.46	0.50
1:A:362:LEU:HA	1:A:472:ASN:HD22	1.77	0.50
1:A:1076:GLU:C	1:A:1078:ALA:H	2.19	0.50
2:B:797:TYR:C	2:B:798:TYR:HD2	2.20	0.50
2:B:847:ASP:C	2:B:849:GLY:H	2.19	0.50
8:H:109:ASP:OD1	8:H:109:ASP:N	2.45	0.50
10:J:63:ASN:HB3	10:J:64:PRO:HD3	1.93	0.50
1:A:70:CYS:O	1:A:72:GLU:HG2	2.12	0.50
1:A:669:ASP:HB3	1:A:744:VAL:HG23	1.92	0.50
1:A:1128:LEU:HA	1:A:1307:TRP:CD1	2.47	0.50
1:A:1452:LEU:C	1:A:1454:THR:H	2.20	0.50
2:B:875:GLU:HG3	2:B:877:PRO:HD3	1.93	0.50
4:D:65:LYS:O	4:D:69:ARG:HG3	2.12	0.50
1:A:117:GLU:CD	1:A:117:GLU:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:VAL:HG23	8:H:78:TRP:H	1.77	0.49
1:A:1244:VAL:HG12	1:A:1245:ILE:H	1.75	0.49
2:B:220:ALA:HB1	2:B:222:PRO:HD2	1.93	0.49
2:B:394:PHE:HA	2:B:397:LYS:HG3	1.94	0.49
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.12	0.49
1:A:375:LEU:HD13	1:A:492:VAL:HG21	1.93	0.49
1:A:853:TYR:CD1	6:F:136:ARG:HB3	2.47	0.49
2:B:376:ASN:O	2:B:380:LEU:HD13	2.12	0.49
8:H:36:ILE:HA	8:H:125:GLU:O	2.12	0.49
8:H:39:THR:HB	8:H:123:CYS:HB3	1.94	0.49
1:A:764:ALA:O	1:A:804:SER:HB3	2.12	0.49
10:J:56:ILE:HA	10:J:59:PHE:HD2	1.76	0.49
1:A:253:MET:O	1:A:254:ASP:HB2	2.11	0.49
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.43	0.49
7:G:26:LEU:HD12	7:G:56:VAL:HG11	1.95	0.49
11:K:53:TYR:C	11:K:55:ASP:H	2.19	0.49
1:A:266:LYS:HA	1:A:269:ASP:HB2	1.94	0.49
1:A:976:ASP:C	1:A:978:ALA:H	2.19	0.49
2:B:1065:GLN:HE21	2:B:1067:ARG:N	2.10	0.49
5:E:134:PHE:HD2	5:E:139:LEU:HD21	1.78	0.49
5:E:177:ILE:HG22	5:E:212:ILE:O	2.13	0.49
2:B:575:VAL:HA	2:B:619:ILE:HB	1.93	0.49
1:A:1444:PHE:CE2	6:F:89:GLU:HG2	2.48	0.49
2:B:208:ARG:HD2	2:B:208:ARG:O	2.13	0.49
2:B:311:GLU:O	2:B:314:PHE:HB3	2.12	0.49
2:B:489:ARG:HB3	2:B:489:ARG:HH11	1.78	0.49
2:B:1016:ALA:O	2:B:1020:ARG:HG3	2.11	0.49
7:G:34:VAL:O	7:G:37:THR:OG1	2.24	0.49
9:I:7:CYS:HB2	9:I:34:TYR:CE1	2.48	0.49
1:A:458:ALA:HB2	1:A:502:LEU:HD22	1.94	0.49
1:A:519:LYS:HE2	1:A:625:SER:O	2.11	0.49
1:A:768:GLN:HA	1:A:800:PHE:HA	1.95	0.49
1:A:780:PHE:HE2	2:B:510:THR:CG2	2.25	0.49
2:B:399:LEU:HD12	2:B:538:ILE:HD11	1.95	0.49
5:E:31:GLN:HE21	5:E:35:ASP:CG	2.21	0.49
5:E:39:GLU:C	5:E:41:PHE:H	2.19	0.49
8:H:38:LEU:HD11	8:H:122:MET:HE2	1.94	0.49
1:A:283:ASP:O	1:A:285:SER:N	2.46	0.49
1:A:307:ASN:HD21	1:A:315:ALA:HB3	1.77	0.49
1:A:535:MET:O	1:A:575:GLY:HA3	2.13	0.49
2:B:86:ARG:HB3	2:B:87:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:156:SER:C	5:E:158:GLY:H	2.21	0.49
2:B:699:MET:O	2:B:739:THR:OG1	2.27	0.49
11:K:10:PHE:N	11:K:10:PHE:CD2	2.81	0.49
1:A:941:ARG:HH11	1:A:941:ARG:HG2	1.78	0.48
1:A:1321:ALA:HA	5:E:13:ARG:NH2	2.27	0.48
2:B:393:HIS:O	2:B:395:GLY:N	2.46	0.48
2:B:998:ASP:OD1	3:C:34:ARG:NH2	2.46	0.48
3:C:111:THR:O	3:C:147:LEU:HD23	2.13	0.48
1:A:1351:LEU:HD23	1:A:1375:VAL:HG13	1.95	0.48
2:B:190:MET:SD	2:B:190:MET:N	2.87	0.48
3:C:97:VAL:O	3:C:98:LEU:HD23	2.13	0.48
4:D:158:THR:HG22	4:D:159:LEU:HD23	1.94	0.48
5:E:160:LYS:C	5:E:162:GLN:H	2.19	0.48
8:H:98:GLY:HA3	8:H:117:PHE:HA	1.95	0.48
1:A:34:LYS:HD3	1:A:34:LYS:N	2.29	0.48
1:A:89:PRO:C	1:A:204:THR:HG21	2.37	0.48
1:A:715:PHE:HB2	9:I:97:MET:HE1	1.95	0.48
1:A:742:ASN:HD22	1:A:743:ASN:N	2.11	0.48
1:A:807:ARG:NH1	2:B:726:ILE:HG13	2.28	0.48
2:B:428:CYS:C	2:B:430:GLU:H	2.20	0.48
1:A:328:ALA:C	1:A:330:LEU:H	2.21	0.48
1:A:669:ASP:CG	1:A:743:ASN:HD22	2.22	0.48
1:A:828:THR:HA	1:A:831:LYS:HE2	1.94	0.48
2:B:503:LYS:HG2	2:B:504:PRO:CD	2.42	0.48
4:D:114:ARG:NH1	4:D:148:LEU:O	2.46	0.48
4:D:172:GLN:HA	4:D:175:LEU:HD12	1.96	0.48
5:E:90:LYS:C	5:E:92:MET:N	2.71	0.48
5:E:112:GLN:HA	5:E:136:GLU:HG3	1.95	0.48
7:G:51:GLY:O	7:G:54:ILE:HG13	2.13	0.48
1:A:402:GLY:O	1:A:436:HIS:HD2	1.97	0.48
1:A:1241:ARG:HH12	1:A:1243:ARG:HH12	1.61	0.48
2:B:52:GLU:HG3	2:B:53:GLU:N	2.24	0.48
2:B:344:TYR:O	2:B:347:ASP:HB2	2.14	0.48
2:B:1104:HIS:NE2	2:B:1126:GLY:O	2.46	0.48
3:C:51:LYS:O	12:L:62:ARG:NE	2.46	0.48
5:E:123:ILE:C	5:E:125:THR:H	2.21	0.48
10:J:46:ARG:HG2	10:J:46:ARG:NH1	2.28	0.48
2:B:208:ARG:NH1	2:B:400:ASP:OD2	2.47	0.48
2:B:551:LEU:HD23	2:B:589:LEU:HD11	1.96	0.48
2:B:1001:PHE:O	2:B:1072:MET:HA	2.14	0.48
2:B:1177:LYS:O	2:B:1179:GLN:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1196:ILE:HB	2:B:1197:PRO:HD2	1.96	0.48
7:G:6:ASP:HB3	7:G:73:LYS:HZ3	1.79	0.48
9:I:69:PRO:O	9:I:84:VAL:HG23	2.14	0.48
1:A:794:SER:HB2	1:A:795:PRO:HD2	1.94	0.48
1:A:859:ASN:ND2	1:A:861:LEU:H	2.11	0.48
1:A:965:ILE:HA	1:A:968:ASN:HD22	1.79	0.48
2:B:800:GLN:CG	10:J:51:THR:HG22	2.39	0.48
3:C:236:GLY:O	3:C:238:LEU:N	2.47	0.48
9:I:50:THR:HG22	9:I:52:ILE:H	1.79	0.48
11:K:90:ALA:O	11:K:94:ILE:HG13	2.14	0.48
1:A:357:ASP:HB2	1:A:470:ARG:NH1	2.29	0.48
1:A:467:SER:CB	11:K:2:ASN:HD22	2.27	0.48
1:A:536:THR:HG21	1:A:617:VAL:HA	1.95	0.48
1:A:1128:LEU:HA	1:A:1307:TRP:HD1	1.78	0.48
1:A:1354:GLU:O	1:A:1358:VAL:HG23	2.13	0.48
2:B:539:SER:HG	2:B:624:GLY:H	1.60	0.48
9:I:14:LEU:HD13	9:I:28:SER:O	2.14	0.48
1:A:231:ARG:HG3	1:A:234:TRP:CH2	2.49	0.48
1:A:1397:THR:HG22	1:A:1398:GLY:N	2.27	0.48
2:B:999:MET:HE2	2:B:1011:ILE:HD11	1.96	0.48
1:A:452:HIS:NE2	1:A:1076:GLU:HG3	2.29	0.47
1:A:505:LEU:HD11	6:F:91:ALA:CB	2.44	0.47
1:A:1335:PHE:N	1:A:1335:PHE:HD2	2.12	0.47
2:B:369:PHE:HB3	2:B:579:TRP:HZ3	1.79	0.47
5:E:123:ILE:CG1	5:E:124:PRO:HD3	2.44	0.47
8:H:90:ASP:C	8:H:92:TYR:H	2.21	0.47
2:B:519:GLU:HA	2:B:771:SER:HB3	1.97	0.47
2:B:882:THR:HG22	2:B:884:ARG:H	1.80	0.47
1:A:93:ILE:CG2	1:A:302:ALA:HA	2.41	0.47
1:A:389:LEU:O	1:A:393:VAL:HG23	2.15	0.47
1:A:1264:LYS:O	1:A:1267:GLU:HB3	2.14	0.47
1:A:1335:PHE:N	1:A:1335:PHE:CD2	2.82	0.47
1:A:1389:ARG:HD2	1:A:1390:HIS:CE1	2.50	0.47
2:B:901:PRO:HA	2:B:949:VAL:HB	1.96	0.47
4:D:171:LEU:HA	4:D:174:ILE:HD12	1.95	0.47
1:A:276:ASN:O	1:A:280:LEU:HG	2.15	0.47
1:A:321:ARG:NH2	1:A:324:LYS:HE3	2.29	0.47
1:A:549:ASN:OD1	11:K:61:TYR:HD2	1.98	0.47
2:B:300:TRP:CH2	9:I:45:ARG:HB3	2.49	0.47
2:B:701:ALA:HB2	2:B:738:PHE:HD2	1.78	0.47
2:B:744:HIS:ND1	2:B:745:PRO:HD2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1096:ARG:HA	2:B:1098:MET:HE2	1.97	0.47
4:D:48:LEU:HD13	4:D:49:ILE:H	1.80	0.47
1:A:226:ASN:ND2	1:A:229:TYR:H	2.02	0.47
1:A:755:SER:H	1:A:758:ASN:HD22	1.62	0.47
1:A:1444:PHE:HE1	6:F:92:ARG:HD3	1.80	0.47
1:A:1444:PHE:CZ	6:F:89:GLU:HA	2.49	0.47
2:B:1202:LEU:O	2:B:1206:GLU:HG3	2.15	0.47
5:E:143:ILE:O	5:E:149:VAL:HG21	2.15	0.47
6:F:118:LEU:O	6:F:122:MET:HG3	2.14	0.47
1:A:395:ASN:O	1:A:399:GLU:HB2	2.14	0.47
1:A:606:MET:HG2	1:A:622:THR:HG21	1.96	0.47
1:A:606:MET:HE3	1:A:607:LEU:H	1.79	0.47
1:A:1300:GLU:HG3	1:A:1300:GLU:H	1.40	0.47
1:A:1447:MET:HE1	6:F:135:ARG:HB2	1.96	0.47
2:B:825:VAL:HG21	2:B:1090:THR:HB	1.94	0.47
3:C:184:ASN:ND2	3:C:189:THR:HB	2.28	0.47
1:A:185:THR:HA	1:A:198:PRO:O	2.15	0.47
1:A:448:GLN:HA	1:A:449:PRO:C	2.40	0.47
1:A:598:LEU:HD22	8:H:114:TYR:CE1	2.49	0.47
1:A:839:GLN:O	1:A:843:VAL:HG23	2.15	0.47
2:B:166:ARG:HG3	2:B:166:ARG:HH11	1.78	0.47
2:B:851:PHE:O	2:B:974:PRO:HD3	2.14	0.47
2:B:1176:LYS:C	2:B:1178:ASN:H	2.23	0.47
2:B:1177:LYS:C	2:B:1179:GLN:H	2.23	0.47
3:C:201:TRP:HE3	3:C:202:PRO:HD2	1.80	0.47
1:A:846:LEU:HB3	1:A:849:ILE:HD12	1.96	0.47
2:B:756:ILE:O	2:B:759:PRO:HD3	2.15	0.47
2:B:851:PHE:O	2:B:1094:ARG:NH1	2.47	0.47
7:G:74:TYR:H	7:G:74:TYR:HD2	1.63	0.47
1:A:519:LYS:HB2	1:A:520:PRO:HD2	1.97	0.47
1:A:1210:THR:O	1:A:1214:VAL:HG23	2.15	0.47
1:A:1282:ILE:HD11	1:A:1315:ASN:HB3	1.97	0.47
1:A:1439:MET:O	2:B:1144:ALA:HB2	2.15	0.47
2:B:551:LEU:O	2:B:553:GLU:N	2.43	0.47
2:B:630:LEU:HD22	2:B:741:CYS:O	2.15	0.47
4:D:166:LYS:O	4:D:167:LYS:HB2	2.14	0.47
6:F:125:LEU:HG	6:F:153:VAL:HG11	1.97	0.47
7:G:39:THR:O	7:G:43:GLY:N	2.46	0.47
1:A:110:CYS:SG	1:A:111:GLY:N	2.87	0.47
1:A:831:LYS:HZ3	1:A:1082:THR:HG23	1.79	0.47
1:A:962:LEU:HA	1:A:965:ILE:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1400:LEU:HB2	1:A:1429:GLU:OE1	2.15	0.47
1:A:1447:MET:HB2	1:A:1447:MET:HE3	1.67	0.47
2:B:476:LEU:HD11	2:B:484:THR:HG23	1.97	0.47
2:B:550:PHE:HD2	2:B:550:PHE:O	1.98	0.47
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.40	0.47
4:D:177:GLU:HA	4:D:180:ARG:HB2	1.97	0.47
1:A:134:ARG:NH1	1:A:224:GLY:HA2	2.30	0.46
1:A:656:TYR:O	1:A:659:LEU:HB3	2.15	0.46
1:A:766:VAL:HG23	1:A:803:ASN:O	2.15	0.46
2:B:405:LEU:HB3	2:B:459:TRP:HZ2	1.80	0.46
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	1.97	0.46
3:C:47:LEU:HB3	3:C:158:ILE:CG1	2.45	0.46
7:G:95:SER:O	7:G:130:TYR:OH	2.22	0.46
10:J:20:ALA:O	10:J:24:LEU:HG	2.15	0.46
1:A:495:SER:O	1:A:499:ARG:HG3	2.16	0.46
1:A:988:ILE:O	1:A:992:VAL:HG23	2.15	0.46
7:G:120:VAL:O	7:G:131:MET:N	2.39	0.46
8:H:41:ASP:O	8:H:42:ILE:HG13	2.14	0.46
11:K:65:HIS:HD2	11:K:67:LEU:HB2	1.80	0.46
1:A:50:GLU:C	1:A:52:GLY:H	2.24	0.46
1:A:362:LEU:HA	1:A:472:ASN:ND2	2.31	0.46
1:A:415:ASP:OD1	1:A:417:ARG:HG2	2.16	0.46
1:A:752:SER:O	1:A:753:LYS:HG2	2.15	0.46
1:A:761:GLN:HA	1:A:766:VAL:HA	1.97	0.46
1:A:782:ASP:CG	9:I:91:ARG:HH22	2.23	0.46
2:B:459:TRP:HA	2:B:459:TRP:CE3	2.50	0.46
2:B:865:ARG:CG	2:B:871:VAL:HG22	2.45	0.46
1:A:601:PRO:C	1:A:603:ASP:H	2.23	0.46
1:A:808:GLY:HA2	2:B:760:ASP:O	2.15	0.46
3:C:168:ALA:C	3:C:170:TRP:H	2.24	0.46
4:D:179:ASN:HA	4:D:182:GLU:HB2	1.97	0.46
5:E:120:ASN:C	5:E:122:MET:H	2.23	0.46
1:A:78:PRO:HA	2:B:1201:LYS:NZ	2.30	0.46
3:C:167:HIS:HD2	3:C:168:ALA:H	1.64	0.46
5:E:84:GLU:O	5:E:86:SER:N	2.44	0.46
9:I:74:GLU:O	9:I:74:GLU:HG3	2.14	0.46
1:A:212:PHE:HB3	1:A:233:GLU:HB3	1.98	0.46
1:A:593:ASP:H	1:A:596:ASN:CG	2.24	0.46
1:A:601:PRO:HA	8:H:25:ARG:NH1	2.30	0.46
1:A:936:GLN:O	1:A:939:SER:N	2.49	0.46
2:B:612:ILE:O	2:B:614:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1167:GLY:O	2:B:1168:LEU:HD23	2.15	0.46
4:D:163:LEU:HA	4:D:166:LYS:HB2	1.97	0.46
8:H:88:LEU:C	8:H:90:ASP:N	2.74	0.46
10:J:23:ARG:C	10:J:25:LEU:N	2.73	0.46
1:A:570:LYS:O	1:A:572:LEU:HD12	2.16	0.46
2:B:572:ARG:HB2	2:B:579:TRP:HE1	1.80	0.46
2:B:766:ARG:HH22	2:B:1020:ARG:NH1	2.10	0.46
2:B:997:GLU:CD	2:B:997:GLU:H	2.22	0.46
3:C:242:GLN:C	3:C:244:PHE:H	2.23	0.46
6:F:97:ARG:O	6:F:101:ILE:HG13	2.16	0.46
1:A:270:ILE:HG12	1:A:300:HIS:HB3	1.98	0.46
1:A:386:ILE:HG22	1:A:387:HIS:N	2.30	0.46
1:A:574:THR:O	1:A:577:GLN:HB2	2.15	0.46
1:A:853:TYR:HB3	6:F:81:THR:HG22	1.97	0.46
1:A:1449:ASP:HB3	1:A:1452:LEU:CG	2.46	0.46
2:B:1172:ILE:O	2:B:1172:ILE:HG22	2.15	0.46
7:G:89:ALA:HB2	7:G:103:VAL:HG22	1.98	0.46
9:I:78:CYS:HG	9:I:80:SER:HG	1.57	0.46
1:A:80:HIS:O	1:A:244:PRO:HB3	2.15	0.46
1:A:447:ARG:HD3	1:A:479:TYR:HB3	1.97	0.46
1:A:504:GLN:NE2	6:F:90:ARG:HH21	2.14	0.46
1:A:1142:TYR:HA	1:A:1278:GLY:HA3	1.98	0.46
2:B:481:TYR:O	2:B:485:LEU:HG	2.16	0.46
2:B:609:ILE:N	2:B:609:ILE:HD12	2.30	0.46
2:B:955:THR:O	2:B:963:PHE:N	2.35	0.46
3:C:100:LEU:HD22	3:C:118:LEU:HD21	1.98	0.46
5:E:28:PHE:O	5:E:29:ILE:HG13	2.16	0.46
7:G:166:ASP:O	7:G:168:LEU:HG	2.15	0.46
1:A:358:PRO:HD2	2:B:833:TYR:CE1	2.51	0.45
2:B:409:LEU:HD12	2:B:459:TRP:CE2	2.51	0.45
2:B:607:SER:OG	2:B:620:PHE:HB2	2.16	0.45
7:G:122:ASN:OD1	7:G:125:ASN:HB3	2.15	0.45
1:A:762:MET:HA	1:A:805:TYR:HB2	1.98	0.45
1:A:958:LEU:HD13	1:A:1023:LEU:HD22	1.97	0.45
2:B:835:GLN:HE21	2:B:835:GLN:HB2	1.57	0.45
8:H:90:ASP:O	8:H:92:TYR:N	2.42	0.45
1:A:55:ASP:C	1:A:57:LYS:H	2.23	0.45
1:A:842:LEU:O	1:A:846:LEU:HG	2.16	0.45
1:A:1322:VAL:O	1:A:1325:VAL:HG22	2.17	0.45
1:A:1444:PHE:CD1	1:A:1444:PHE:C	2.94	0.45
2:B:421:ILE:O	2:B:425:MET:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:824:ILE:HG22	2:B:1087:PHE:HE2	1.81	0.45
2:B:843:GLN:N	2:B:994:TYR:O	2.47	0.45
2:B:945:GLU:O	2:B:946:ASN:HB3	2.17	0.45
2:B:955:THR:N	2:B:963:PHE:O	2.49	0.45
4:D:122:THR:O	4:D:126:GLN:HG3	2.17	0.45
8:H:12:VAL:HG13	8:H:26:ILE:HG23	1.97	0.45
11:K:43:ALA:HB1	11:K:61:TYR:CD1	2.51	0.45
1:A:501:GLU:OE2	1:A:1441:THR:HG21	2.16	0.45
1:A:576:LYS:HE2	1:A:616:GLY:O	2.16	0.45
2:B:326:ILE:HG22	2:B:326:ILE:O	2.15	0.45
2:B:702:MET:HA	2:B:702:MET:HE3	1.97	0.45
3:C:257:ASN:HA	3:C:260:PHE:HB3	1.99	0.45
11:K:70:ASN:O	11:K:71:PHE:HB3	2.15	0.45
2:B:466:MET:C	2:B:468:SER:H	2.25	0.45
2:B:752:ALA:HB1	2:B:771:SER:HA	1.97	0.45
8:H:19:ARG:C	8:H:20:TYR:HD2	2.24	0.45
1:A:712:ARG:O	1:A:715:PHE:HB3	2.17	0.45
2:B:108:ASN:OD1	2:B:860:MET:HE2	2.16	0.45
2:B:477:ASN:O	2:B:478:ARG:HD2	2.17	0.45
2:B:596:LEU:HD13	2:B:601:ALA:HB3	1.98	0.45
2:B:913:GLY:HA2	2:B:938:SER:OG	2.17	0.45
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.65	0.45
4:D:48:LEU:CD1	4:D:49:ILE:H	2.29	0.45
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.98	0.45
1:A:467:SER:HB2	2:B:1099:VAL:HG11	1.97	0.45
1:A:869:TYR:CD2	1:A:1060:VAL:HG21	2.51	0.45
2:B:101:PRO:O	2:B:103:GLU:N	2.49	0.45
2:B:266:PRO:O	2:B:267:TYR:HB2	2.16	0.45
2:B:514:LEU:HB3	2:B:626:VAL:HG11	1.98	0.45
3:C:39:GLU:HG2	3:C:165:LYS:HE3	1.99	0.45
4:D:169:VAL:C	4:D:171:LEU:N	2.74	0.45
1:A:107:CYS:HA	1:A:172:GLN:OE1	2.17	0.45
1:A:762:MET:HG2	1:A:805:TYR:HD1	1.81	0.45
1:A:1173:GLU:C	1:A:1175:TYR:H	2.25	0.45
2:B:344:TYR:CE2	2:B:348:ILE:HD11	2.52	0.45
5:E:166:ARG:HA	5:E:166:ARG:HD3	1.85	0.45
6:F:109:VAL:HG12	6:F:110:ASP:N	2.21	0.45
1:A:634:VAL:HG12	1:A:643:CYS:HB2	1.98	0.45
1:A:744:VAL:O	1:A:748:VAL:HG23	2.17	0.45
1:A:1440:GLY:O	1:A:1442:GLY:N	2.50	0.45
2:B:1201:LYS:HG2	2:B:1202:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:41:HIS:HB2	7:G:73:LYS:NZ	2.30	0.45
4:D:169:VAL:O	4:D:171:LEU:N	2.50	0.45
7:G:35:GLU:HG2	7:G:48:VAL:HG23	1.99	0.45
7:G:143:VAL:HA	7:G:170:ALA:HA	1.98	0.45
1:A:357:ASP:OD2	11:K:65:HIS:CE1	2.66	0.45
2:B:555:GLY:HA3	2:B:583:HIS:HE1	1.82	0.45
2:B:1001:PHE:CE1	3:C:178:PHE:HB3	2.52	0.45
3:C:167:HIS:CD2	3:C:168:ALA:H	2.35	0.45
4:D:51:LEU:O	7:G:2:PHE:HB2	2.17	0.45
5:E:170:LYS:O	5:E:172:SER:N	2.48	0.45
7:G:40:GLY:HA2	7:G:157:ILE:HD11	1.99	0.45
1:A:105:CYS:SG	1:A:139:TRP:HA	2.57	0.44
1:A:354:ILE:CG2	1:A:488:MET:HG3	2.46	0.44
1:A:1295:PRO:HG3	1:A:1301:TYR:CZ	2.52	0.44
1:A:1403:CYS:HB2	1:A:1412:LEU:HD21	2.00	0.44
2:B:509:ASN:N	2:B:509:ASN:ND2	2.59	0.44
2:B:550:PHE:CE1	2:B:596:LEU:HG	2.51	0.44
2:B:745:PRO:O	2:B:748:ILE:HG12	2.17	0.44
3:C:81:TYR:HE2	3:C:162:GLY:H	1.64	0.44
4:D:114:ARG:HH21	4:D:182:GLU:CD	2.26	0.44
5:E:196:LYS:HE2	5:E:198:ILE:HD11	1.99	0.44
1:A:801:VAL:HG22	1:A:813:GLU:HB3	1.98	0.44
1:A:1085:THR:O	1:A:1085:THR:HG22	2.16	0.44
1:A:1326:ASP:OD1	1:A:1328:SER:HB2	2.17	0.44
2:B:863:GLU:OE1	2:B:962:LYS:HB2	2.17	0.44
9:I:100:PHE:N	9:I:100:PHE:CD1	2.85	0.44
1:A:67:CYS:O	1:A:70:CYS:SG	2.76	0.44
1:A:72:GLU:OE2	2:B:1175:LEU:HB2	2.18	0.44
1:A:356:GLY:HA2	1:A:471:LEU:O	2.17	0.44
1:A:629:GLY:O	1:A:633:THR:HG23	2.17	0.44
1:A:843:VAL:C	1:A:845:ALA:H	2.26	0.44
2:B:761:HIS:HB2	2:B:1024:ALA:HB2	2.00	0.44
2:B:774:GLY:C	2:B:776:GLN:H	2.26	0.44
2:B:890:TYR:O	2:B:893:LEU:HB2	2.17	0.44
1:A:447:ARG:CD	1:A:481:ALA:HB2	2.48	0.44
1:A:786:PRO:HG2	1:A:787:HIS:CD2	2.53	0.44
2:B:992:VAL:HG22	2:B:993:THR:N	2.33	0.44
3:C:42:THR:HG22	3:C:43:LEU:N	2.24	0.44
3:C:147:LEU:HA	10:J:60:LEU:CD2	2.46	0.44
4:D:41:HIS:ND1	4:D:41:HIS:C	2.75	0.44
1:A:340:ASN:O	1:A:344:LYS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1214:VAL:O	1:A:1218:ILE:HG13	2.18	0.44
2:B:1151:LEU:HD13	2:B:1151:LEU:H	1.82	0.44
3:C:166:GLU:HB3	3:C:170:TRP:CZ3	2.52	0.44
8:H:61:ASN:O	8:H:62:SER:HB2	2.18	0.44
1:A:269:ASP:HB3	1:A:300:HIS:CE1	2.53	0.44
1:A:386:ILE:O	1:A:390:THR:OG1	2.34	0.44
1:A:601:PRO:HG2	1:A:602:LYS:H	1.83	0.44
2:B:414:PHE:HA	2:B:417:LEU:HB3	1.99	0.44
2:B:596:LEU:HD22	2:B:596:LEU:HA	1.86	0.44
2:B:632:ILE:HG22	2:B:634:GLU:HG2	2.00	0.44
2:B:883:LEU:O	2:B:885:LEU:N	2.51	0.44
4:D:67:ARG:C	4:D:69:ARG:H	2.26	0.44
1:A:445:PHE:CE2	1:A:488:MET:HE3	2.53	0.44
1:A:1222:PHE:CG	1:A:1226:LEU:HD23	2.52	0.44
2:B:164:MET:HE2	2:B:192:GLY:O	2.17	0.44
2:B:286:ASP:CG	9:I:12:ASN:HA	2.43	0.44
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.83	0.44
3:C:5:PRO:HA	3:C:23:ASP:HB3	2.00	0.44
7:G:127:PRO:HG2	7:G:138:THR:HG21	2.00	0.44
1:A:312:GLN:O	1:A:313:PRO:C	2.61	0.44
1:A:1367:ASN:HD22	1:A:1368:TYR:H	1.66	0.44
2:B:381:CYS:C	2:B:383:LEU:H	2.25	0.44
5:E:14:SER:HA	5:E:140:VAL:HA	1.98	0.44
6:F:76:LYS:O	6:F:79:ARG:HD3	2.18	0.44
10:J:59:PHE:HA	10:J:62:TYR:HD1	1.83	0.44
1:A:14:VAL:HG21	2:B:1216:LEU:HD12	1.99	0.44
1:A:41:MET:HE3	1:A:42:ASP:N	2.32	0.44
1:A:262:ASP:OD1	1:A:323:VAL:HA	2.18	0.44
1:A:886:THR:HG22	1:A:941:ARG:HD2	2.00	0.44
1:A:1444:PHE:CE2	6:F:89:GLU:HA	2.53	0.44
2:B:157:HIS:C	2:B:158:ILE:HG13	2.42	0.44
5:E:77:LEU:HA	5:E:106:THR:HB	2.00	0.44
7:G:121:TYR:HA	7:G:130:TYR:HA	1.98	0.44
2:B:549:ASN:O	2:B:551:LEU:N	2.51	0.43
2:B:698:ILE:HD11	2:B:700:ILE:HD11	2.00	0.43
2:B:1080:LYS:HG3	3:C:180:TYR:CE2	2.53	0.43
3:C:213:PRO:O	3:C:214:LYS:HB2	2.18	0.43
6:F:89:GLU:O	6:F:93:ILE:HG13	2.18	0.43
1:A:297:LEU:O	1:A:301:VAL:HG23	2.18	0.43
1:A:328:ALA:C	1:A:330:LEU:N	2.76	0.43
1:A:379:GLU:OE1	1:A:435:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:ILE:HD12	1:A:668:GLY:H	1.83	0.43
1:A:827:ASP:O	1:A:831:LYS:N	2.43	0.43
1:A:1032:ARG:HH11	1:A:1032:ARG:HB3	1.83	0.43
1:A:1096:VAL:HA	1:A:1115:THR:HG21	2.00	0.43
2:B:612:ILE:C	2:B:614:GLU:N	2.77	0.43
2:B:914:LYS:HG2	2:B:937:ALA:HB3	2.01	0.43
2:B:1060:ARG:NH2	3:C:199:LYS:O	2.42	0.43
2:B:1073:TYR:OH	3:C:179:GLU:HA	2.18	0.43
5:E:115:ILE:HG22	5:E:119:ALA:HB3	2.00	0.43
5:E:160:LYS:C	5:E:162:GLN:N	2.76	0.43
1:A:12:ARG:HE	2:B:1192:TYR:HE2	1.65	0.43
1:A:73:GLY:O	1:A:75:ALA:N	2.51	0.43
1:A:897:ARG:HD3	1:A:898:TYR:CE1	2.52	0.43
1:A:1149:THR:O	9:I:48:LEU:HB2	2.18	0.43
2:B:16:ASP:C	2:B:18:TRP:N	2.77	0.43
2:B:1162:VAL:HG12	2:B:1163:CYS:N	2.32	0.43
4:D:25:ALA:C	4:D:27:LEU:H	2.25	0.43
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.78	0.43
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.53	0.43
7:G:114:LEU:HB3	7:G:162:SER:HB3	2.00	0.43
1:A:382:THR:C	1:A:384:TYR:H	2.27	0.43
1:A:568:LYS:HD3	8:H:94:TYR:HA	1.99	0.43
1:A:859:ASN:HD22	1:A:861:LEU:H	1.66	0.43
1:A:1288:VAL:O	1:A:1308:ALA:N	2.46	0.43
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.53	0.43
2:B:999:MET:HE2	2:B:1011:ILE:CD1	2.48	0.43
7:G:154:VAL:HB	7:G:155:ASN:H	1.57	0.43
1:A:264:THR:HG22	1:A:264:THR:O	2.19	0.43
1:A:336:ARG:CA	1:A:340:ASN:HD22	2.28	0.43
1:A:580:SER:HB3	1:A:612:LYS:HA	2.01	0.43
1:A:1426:GLY:O	1:A:1429:GLU:HG2	2.18	0.43
2:B:211:ALA:O	2:B:213:ILE:HG13	2.17	0.43
2:B:572:ARG:HG2	2:B:572:ARG:HH11	1.83	0.43
2:B:947:GLY:C	2:B:948:ILE:HG13	2.44	0.43
2:B:950:ASP:O	2:B:951:GLN:HB2	2.18	0.43
3:C:85:CYS:C	3:C:87:CYS:H	2.26	0.43
11:K:48:GLU:C	11:K:50:LEU:H	2.27	0.43
1:A:226:ASN:HD21	1:A:228:ASP:HB3	1.83	0.43
1:A:768:GLN:NE2	1:A:798:LYS:O	2.45	0.43
1:A:856:THR:HG21	1:A:858:ARG:NE	2.32	0.43
1:A:986:PRO:O	1:A:990:HIS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1097:THR:HG21	1:A:1114:LYS:HB2	2.01	0.43
10:J:52:HIS:CD2	10:J:53:VAL:N	2.87	0.43
1:A:588:HIS:CD2	1:A:967:GLN:HB3	2.54	0.43
1:A:723:LEU:HB3	1:A:800:PHE:CE1	2.54	0.43
1:A:831:LYS:NZ	1:A:1082:THR:HA	2.34	0.43
1:A:872:ASP:OD2	1:A:874:LEU:HB2	2.18	0.43
1:A:988:ILE:HG22	1:A:989:ILE:N	2.34	0.43
2:B:252:ARG:C	2:B:254:ASP:H	2.26	0.43
2:B:724:LYS:HG2	2:B:1051:THR:HG21	2.00	0.43
1:A:347:ASP:OD1	2:B:1106:ARG:NE	2.44	0.43
1:A:561:VAL:CG2	8:H:78:TRP:H	2.32	0.43
1:A:1444:PHE:C	1:A:1444:PHE:HD1	2.27	0.43
2:B:785:TYR:CE2	10:J:59:PHE:CE1	3.03	0.43
2:B:847:ASP:HB3	3:C:167:HIS:NE2	2.33	0.43
5:E:15:PHE:CZ	5:E:19:LYS:HE2	2.54	0.43
7:G:43:GLY:HA3	7:G:80:LYS:HB3	2.00	0.43
9:I:61:ASP:C	9:I:63:GLY:H	2.27	0.43
1:A:445:PHE:CZ	1:A:488:MET:HE3	2.54	0.43
1:A:576:LYS:HZ1	1:A:616:GLY:H	1.66	0.43
1:A:1427:VAL:O	1:A:1431:VAL:HG23	2.19	0.43
10:J:8:PHE:H	10:J:48:MET:HE3	1.84	0.43
1:A:933:GLU:OE1	1:A:989:ILE:HG22	2.19	0.43
2:B:484:THR:O	2:B:488:LEU:HD12	2.19	0.43
2:B:794:ASN:C	2:B:795:ILE:HD12	2.43	0.43
4:D:56:SER:O	4:D:60:ILE:HG13	2.19	0.43
8:H:9:ILE:HG12	8:H:56:THR:HG23	2.01	0.43
9:I:33:ASP:O	9:I:35:THR:HG23	2.19	0.43
1:A:32:VAL:HG11	1:A:68:GLN:OE1	2.19	0.42
1:A:373:LYS:HA	1:A:436:HIS:CE1	2.54	0.42
1:A:553:TRP:CD1	11:K:62:LYS:CB	3.01	0.42
1:A:1328:SER:HA	5:E:146:HIS:HA	2.01	0.42
1:A:1393:ASN:HA	1:A:1402:ARG:HG2	2.01	0.42
2:B:342:ILE:O	2:B:345:ALA:HB3	2.19	0.42
2:B:478:ARG:NH2	2:B:782:LEU:HD11	2.33	0.42
2:B:1220:ARG:HB3	2:B:1220:ARG:NH1	2.33	0.42
3:C:221:TYR:CD1	3:C:222:LYS:HG3	2.54	0.42
1:A:454:MET:N	1:A:454:MET:SD	2.93	0.42
1:A:1193:TRP:O	1:A:1243:ARG:HG2	2.19	0.42
2:B:166:ARG:HB2	2:B:191:GLY:HA3	2.01	0.42
2:B:632:ILE:HD12	2:B:685:GLY:O	2.19	0.42
2:B:1157:ALA:O	2:B:1158:PHE:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:252:GLN:NE2	11:K:95:ILE:HG23	2.34	0.42
8:H:107:ASP:O	8:H:108:GLU:C	2.63	0.42
11:K:65:HIS:CD2	11:K:67:LEU:HB2	2.55	0.42
1:A:964:ARG:O	1:A:967:GLN:N	2.52	0.42
1:A:1061:HIS:ND1	6:F:86:THR:HA	2.33	0.42
1:A:1149:THR:HB	9:I:48:LEU:HD12	2.02	0.42
1:A:1211:MET:HB3	1:A:1230:TRP:CD1	2.54	0.42
2:B:305:MET:HE3	2:B:379:LEU:HD22	2.00	0.42
2:B:458:ASN:HD22	2:B:458:ASN:N	2.17	0.42
2:B:702:MET:HB3	2:B:703:THR:H	1.56	0.42
2:B:986:GLN:NE2	2:B:1016:ALA:O	2.52	0.42
2:B:1120:GLU:HG2	2:B:1121:GLY:N	2.34	0.42
4:D:54:SER:HB3	4:D:113:ALA:HB1	2.00	0.42
6:F:81:THR:HB	6:F:136:ARG:HH11	1.85	0.42
1:A:55:ASP:CG	1:A:55:ASP:O	2.62	0.42
1:A:262:ASP:OD2	1:A:321:ARG:NE	2.48	0.42
1:A:783:ARG:HH21	2:B:696:GLU:C	2.25	0.42
1:A:1327:SER:HB2	5:E:141:VAL:HG11	2.00	0.42
2:B:252:ARG:NH1	2:B:252:ARG:HB3	2.34	0.42
2:B:401:LEU:O	2:B:405:LEU:HG	2.18	0.42
2:B:785:TYR:HA	2:B:788:ARG:HG3	2.01	0.42
10:J:3:ILE:HA	10:J:4:PRO:HD3	1.66	0.42
1:A:1294:VAL:HA	1:A:1295:PRO:HD3	1.82	0.42
2:B:91:GLU:OE1	12:L:56:ARG:NH2	2.52	0.42
5:E:12:TRP:O	5:E:15:PHE:HB3	2.19	0.42
12:L:62:ARG:HG2	12:L:63:THR:H	1.84	0.42
1:A:72:GLU:HB3	1:A:76:GLU:HB3	2.01	0.42
1:A:107:CYS:SG	1:A:108:MET:N	2.92	0.42
1:A:475:VAL:HG22	1:A:475:VAL:O	2.20	0.42
1:A:1455:SER:C	1:A:1457:PRO:HD3	2.45	0.42
2:B:202:VAL:HG11	2:B:488:LEU:HA	2.01	0.42
2:B:416:LYS:HB2	2:B:416:LYS:NZ	2.34	0.42
7:G:80:LYS:HE2	7:G:80:LYS:N	2.34	0.42
1:A:55:ASP:N	1:A:56:PRO:CD	2.83	0.42
1:A:329:ARG:O	1:A:336:ARG:HB2	2.19	0.42
1:A:1210:THR:HG22	1:A:1212:ASN:H	1.85	0.42
2:B:549:ASN:C	2:B:551:LEU:N	2.77	0.42
2:B:704:PRO:HG2	2:B:705:GLU:H	1.84	0.42
2:B:1162:VAL:O	2:B:1191:ILE:HG23	2.19	0.42
5:E:14:SER:HA	5:E:139:LEU:O	2.20	0.42
5:E:119:ALA:O	5:E:121:LYS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:123:LYS:HE3	6:F:123:LYS:HB2	1.79	0.42
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.55	0.42
8:H:94:TYR:HE2	8:H:96:MET:HG3	1.85	0.42
9:I:50:THR:HG22	9:I:51:ASN:N	2.30	0.42
1:A:59:GLY:HA2	1:A:67:CYS:HA	2.01	0.42
1:A:147:VAL:O	1:A:149:GLU:N	2.52	0.42
1:A:576:LYS:NZ	1:A:616:GLY:H	2.18	0.42
1:A:689:GLU:HA	1:A:692:GLN:HB3	2.01	0.42
1:A:1413:PHE:C	1:A:1415:ALA:H	2.27	0.42
2:B:279:ARG:NH1	2:B:316:ILE:O	2.52	0.42
2:B:324:ASP:OD1	2:B:341:ARG:NE	2.51	0.42
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.87	0.42
2:B:842:ASN:ND2	2:B:845:SER:OG	2.53	0.42
4:D:169:VAL:C	4:D:171:LEU:H	2.27	0.42
8:H:12:VAL:HG13	8:H:26:ILE:CG2	2.50	0.42
10:J:21:TYR:CE2	10:J:25:LEU:HD11	2.55	0.42
1:A:18:GLN:HG2	1:A:1421:LEU:HD13	2.01	0.42
1:A:278:GLN:C	1:A:280:LEU:H	2.28	0.42
1:A:316:LEU:HD22	1:A:322:PRO:HA	2.01	0.42
2:B:298:ASN:ND2	9:I:3:SER:OG	2.53	0.42
2:B:549:ASN:C	2:B:551:LEU:H	2.28	0.42
2:B:598:ARG:NH2	2:B:688:GLU:OE1	2.53	0.42
7:G:138:THR:O	7:G:141:SER:OG	2.37	0.42
10:J:3:ILE:HG22	10:J:52:HIS:CE1	2.54	0.42
12:L:30:LYS:HG3	12:L:41:SER:CB	2.50	0.42
1:A:20:GLY:C	1:A:21:LEU:HD23	2.45	0.42
1:A:69:THR:C	1:A:71:GLY:N	2.75	0.42
1:A:454:MET:HE3	1:A:514:SER:HB2	2.02	0.42
1:A:578:LEU:O	1:A:581:ILE:HG23	2.19	0.42
1:A:615:PHE:CB	8:H:121:LEU:HD21	2.49	0.42
1:A:856:THR:CG2	1:A:858:ARG:HE	2.33	0.42
1:A:1016:ALA:HA	5:E:204:SER:HB2	2.01	0.42
2:B:390:ASP:HB3	2:B:393:HIS:HB2	2.02	0.42
2:B:491:THR:HG22	2:B:530:LYS:HB2	2.02	0.42
2:B:849:GLY:HA2	2:B:852:ARG:HD2	2.02	0.42
2:B:999:MET:HE3	2:B:999:MET:HA	2.02	0.42
2:B:1021:MET:O	2:B:1023:VAL:HG23	2.19	0.42
7:G:10:ILE:HA	7:G:70:PHE:O	2.20	0.42
7:G:49:LEU:O	7:G:50:ASP:C	2.63	0.42
1:A:146:MET:HA	1:A:172:GLN:NE2	2.34	0.41
1:A:601:PRO:HA	8:H:25:ARG:HH12	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1316:LEU:O	1:A:1318:GLU:N	2.53	0.41
2:B:405:LEU:HB3	2:B:459:TRP:CZ2	2.55	0.41
2:B:841:MET:HE1	2:B:980:PHE:CE2	2.55	0.41
3:C:42:THR:HB	3:C:170:TRP:HD1	1.85	0.41
4:D:41:HIS:CD2	7:G:73:LYS:HG2	2.54	0.41
9:I:34:TYR:CD2	9:I:35:THR:N	2.81	0.41
1:A:699:GLN:HB3	9:I:99:LEU:HG	2.02	0.41
1:A:699:GLN:HE21	9:I:99:LEU:HD21	1.84	0.41
1:A:983:LEU:HD13	1:A:988:ILE:HD11	2.02	0.41
2:B:227:HIS:O	2:B:249:LEU:HB3	2.20	0.41
2:B:266:PRO:CG	2:B:352:GLU:HB3	2.49	0.41
2:B:572:ARG:HG2	2:B:572:ARG:H	1.70	0.41
4:D:26:THR:CB	7:G:84:GLY:HA3	2.51	0.41
5:E:72:SER:HB2	5:E:73:ASP:H	1.67	0.41
9:I:26:LEU:HD23	9:I:26:LEU:HA	1.92	0.41
1:A:845:ALA:O	1:A:846:LEU:HD23	2.20	0.41
1:A:1298:SER:O	1:A:1298:SER:OG	2.35	0.41
2:B:252:ARG:HB3	2:B:252:ARG:HH11	1.86	0.41
2:B:458:ASN:N	2:B:458:ASN:ND2	2.68	0.41
2:B:563:ASP:HA	2:B:564:PRO:HD2	1.91	0.41
2:B:629:PRO:O	2:B:630:LEU:HD23	2.21	0.41
8:H:79:ARG:HA	8:H:80:PRO:HD3	1.88	0.41
11:K:90:ALA:HA	11:K:93:SER:HB3	2.02	0.41
1:A:65:PHE:O	1:A:66:LYS:C	2.62	0.41
2:B:246:GLN:O	2:B:264:THR:N	2.37	0.41
2:B:270:GLN:CG	2:B:271:ASP:H	2.27	0.41
2:B:557:GLU:HA	2:B:558:PRO:HD2	1.84	0.41
2:B:792:MET:H	2:B:857:ARG:HA	1.86	0.41
2:B:822:ASN:HA	2:B:1091:TYR:HA	2.03	0.41
7:G:6:ASP:HB3	7:G:73:LYS:NZ	2.35	0.41
7:G:138:THR:CG2	7:G:139:LYS:N	2.81	0.41
1:A:68:GLN:C	1:A:70:CYS:H	2.29	0.41
1:A:316:LEU:CD2	1:A:322:PRO:HA	2.51	0.41
1:A:563:GLN:HA	1:A:564:PRO:HD3	1.88	0.41
1:A:624:GLY:C	1:A:626:GLY:H	2.29	0.41
2:B:519:GLU:OE2	2:B:752:ALA:HB2	2.21	0.41
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	2.02	0.41
7:G:25:TYR:CE2	7:G:29:LYS:HD2	2.55	0.41
8:H:141:ILE:C	8:H:142:LEU:HD12	2.45	0.41
10:J:47:ARG:HE	10:J:48:MET:CE	2.32	0.41
1:A:108:MET:O	1:A:110:CYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1082:THR:HG21	1:A:1084:ASN:HD22	1.85	0.41
1:A:1230:TRP:HD1	1:A:1231:SER:O	2.03	0.41
2:B:550:PHE:HE1	2:B:596:LEU:HG	1.85	0.41
2:B:744:HIS:HD2	2:B:746:SER:OG	2.03	0.41
2:B:797:TYR:HB3	2:B:798:TYR:CD2	2.56	0.41
2:B:969:ARG:HG2	2:B:970:THR:N	2.36	0.41
4:D:138:HIS:O	4:D:140:PHE:N	2.53	0.41
4:D:162:SER:O	4:D:166:LYS:HD2	2.21	0.41
5:E:134:PHE:CZ	5:E:185:ARG:HB3	2.55	0.41
6:F:140:ASP:OD1	6:F:142:SER:OG	2.38	0.41
11:K:6:ARG:O	11:K:9:LEU:HG	2.21	0.41
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.56	0.41
1:A:376:SER:OG	1:A:434:GLU:HB3	2.21	0.41
2:B:89:MET:HB2	2:B:99:MET:HB2	2.03	0.41
2:B:287:GLY:CA	9:I:6:PHE:CE1	3.03	0.41
2:B:572:ARG:HB2	2:B:579:TRP:NE1	2.36	0.41
2:B:830:TYR:HB3	2:B:831:SER:H	1.68	0.41
2:B:1073:TYR:CD1	2:B:1073:TYR:N	2.89	0.41
3:C:161:LYS:HB3	3:C:162:GLY:H	1.58	0.41
6:F:121:ALA:HA	6:F:124:GLU:HB2	2.03	0.41
8:H:20:TYR:HD1	8:H:23:VAL:HB	1.85	0.41
11:K:47:ARG:HB3	11:K:47:ARG:NH1	2.36	0.41
12:L:44:LYS:C	12:L:46:ASP:H	2.28	0.41
1:A:146:MET:HB3	1:A:172:GLN:HB2	2.03	0.41
1:A:263:LEU:C	1:A:265:HIS:N	2.76	0.41
1:A:404:LYS:O	1:A:404:LYS:HG3	2.20	0.41
1:A:895:HIS:C	1:A:897:ARG:H	2.28	0.41
3:C:7:VAL:HG11	11:K:105:PHE:HD1	1.85	0.41
7:G:126:SER:HA	7:G:127:PRO:HA	1.84	0.41
1:A:476:THR:HG23	1:A:477:SER:N	2.35	0.41
1:A:831:LYS:HD2	1:A:1081:MET:O	2.21	0.41
1:A:863:ASP:HA	5:E:173:GLN:HA	2.01	0.41
1:A:1196:ARG:HG3	1:A:1239:ILE:HG23	2.01	0.41
1:A:1371:MET:H	1:A:1371:MET:HE3	1.86	0.41
2:B:416:LYS:NZ	2:B:461:GLU:OE1	2.54	0.41
2:B:679:SER:O	2:B:683:THR:OG1	2.31	0.41
2:B:811:TYR:CD1	2:B:811:TYR:N	2.88	0.41
2:B:812:LEU:C	2:B:814:PHE:N	2.78	0.41
2:B:906:SER:O	2:B:941:LEU:HD23	2.21	0.41
2:B:1095:LEU:H	2:B:1095:LEU:CD1	2.33	0.41
2:B:1115:THR:O	2:B:1116:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	2.03	0.41
3:C:226:ASN:O	3:C:227:ARG:HB2	2.21	0.41
5:E:136:GLU:C	5:E:138:ASP:H	2.28	0.41
10:J:59:PHE:O	10:J:62:TYR:HB2	2.21	0.41
1:A:114:LEU:CD1	1:A:172:GLN:HE22	2.33	0.41
1:A:332:GLY:O	1:A:333:LYS:HB3	2.21	0.41
1:A:333:LYS:H	1:A:338:ARG:HD2	1.86	0.41
1:A:606:MET:HE2	1:A:608:ILE:HG13	2.03	0.41
1:A:961:ASN:OD1	1:A:963:ARG:HB3	2.21	0.41
2:B:466:MET:HE3	2:B:467:SER:CA	2.51	0.41
2:B:493:THR:HA	2:B:494:PRO:HD2	1.76	0.41
2:B:828:ALA:HB2	2:B:1085:VAL:HG13	2.03	0.41
3:C:242:GLN:C	3:C:244:PHE:N	2.79	0.41
11:K:57:THR:H	11:K:77:THR:HA	1.86	0.41
1:A:392:TYR:HA	1:A:401:PRO:O	2.21	0.40
1:A:444:LEU:HD22	1:A:444:LEU:HA	1.91	0.40
1:A:1146:LYS:HB2	1:A:1271:LEU:O	2.20	0.40
1:A:1159:ASP:HA	1:A:1160:PRO:HD2	1.89	0.40
1:A:1279:ILE:CG1	1:A:1282:ILE:HD12	2.51	0.40
2:B:287:GLY:N	2:B:290:LEU:HD23	2.29	0.40
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.56	0.40
5:E:47:ASP:CG	5:E:48:SER:N	2.73	0.40
5:E:153:ILE:HG22	5:E:154:ARG:O	2.21	0.40
9:I:14:LEU:HD12	9:I:27:TYR:HB3	2.02	0.40
9:I:71:SER:HB3	9:I:85:PHE:HE2	1.83	0.40
11:K:24:ASP:OD1	11:K:26:ARG:HB2	2.21	0.40
1:A:785:LEU:HB3	1:A:786:PRO:HD2	2.02	0.40
1:A:1046:TRP:O	1:A:1050:THR:OG1	2.39	0.40
1:A:1155:TYR:HB2	1:A:1194:LEU:HD23	2.02	0.40
2:B:324:ASP:O	2:B:326:ILE:N	2.54	0.40
2:B:573:ILE:O	2:B:579:TRP:HD1	2.05	0.40
2:B:1006:ILE:HG22	10:J:44:CYS:CB	2.49	0.40
2:B:1096:ARG:HD2	2:B:1097:HIS:CE1	2.57	0.40
2:B:1187:ASN:ND2	2:B:1190:ASN:O	2.53	0.40
3:C:131:GLU:HA	3:C:132:PRO:HD3	1.75	0.40
4:D:114:ARG:CZ	4:D:149:GLY:HA2	2.50	0.40
6:F:82:THR:HA	6:F:83:PRO:HD3	1.92	0.40
1:A:366:GLY:HA3	1:A:470:ARG:HB2	2.04	0.40
1:A:768:GLN:HB2	1:A:800:PHE:HD1	1.86	0.40
2:B:466:MET:O	2:B:468:SER:N	2.43	0.40
2:B:705:GLU:HG3	2:B:706:ASP:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:88:ASP:HB3	7:G:144:ARG:HA	2.04	0.40
7:G:89:ALA:HB1	7:G:102:ASP:O	2.21	0.40
8:H:55:LEU:HD23	8:H:145:ARG:OXT	2.21	0.40
12:L:33:CYS:HB3	12:L:36:CYS:O	2.21	0.40
12:L:52:GLU:HB3	12:L:53:CYS:H	1.63	0.40
1:A:134:ARG:HD3	1:A:222:ARG:O	2.22	0.40
1:A:227:GLU:HA	1:A:231:ARG:HG2	2.03	0.40
1:A:598:LEU:N	1:A:598:LEU:HD12	2.36	0.40
1:A:699:GLN:NE2	9:I:99:LEU:HD11	2.37	0.40
1:A:852:HIS:HB2	1:A:856:THR:CG2	2.51	0.40
1:A:1257:ALA:O	1:A:1258:GLU:HB2	2.22	0.40
1:A:1356:LEU:HA	1:A:1359:ILE:HD12	2.03	0.40
2:B:206:GLN:OE1	2:B:472:VAL:HG22	2.21	0.40
2:B:253:GLU:HG2	2:B:253:GLU:O	2.21	0.40
3:C:45:ILE:HA	3:C:159:ALA:HA	2.03	0.40
5:E:169:LEU:C	5:E:170:LYS:HD3	2.47	0.40
8:H:10:PHE:CD1	8:H:10:PHE:N	2.88	0.40
8:H:80:PRO:CB	8:H:81:PRO:HD2	2.52	0.40
11:K:13:PRO:O	11:K:14:ASP:C	2.65	0.40
1:A:759:ILE:H	1:A:759:ILE:HG13	1.60	0.40
1:A:775:ARG:HB2	1:A:798:LYS:HD2	2.04	0.40
1:A:1002:LEU:HD13	1:A:1009:ILE:HG23	2.03	0.40
1:A:1393:ASN:HD21	1:A:1411:ILE:CD1	2.34	0.40
2:B:523:GLY:O	2:B:524:GLN:C	2.64	0.40
5:E:181:ASP:HA	5:E:182:PRO:HD3	1.99	0.40
11:K:6:ARG:C	11:K:8:GLU:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1393/1743 (80%)	972 (70%)	291 (21%)	130 (9%)	0	8
2	B	1055/1227 (86%)	723 (68%)	214 (20%)	118 (11%)	0	6
3	C	259/304 (85%)	186 (72%)	50 (19%)	23 (9%)	0	8
4	D	135/186 (73%)	98 (73%)	23 (17%)	14 (10%)	0	6
5	E	212/214 (99%)	150 (71%)	44 (21%)	18 (8%)	0	9
6	F	82/155 (53%)	58 (71%)	14 (17%)	10 (12%)	0	4
7	G	169/171 (99%)	129 (76%)	27 (16%)	13 (8%)	1	10
8	H	127/145 (88%)	95 (75%)	17 (13%)	15 (12%)	0	4
9	I	111/115 (96%)	71 (64%)	26 (23%)	14 (13%)	0	4
10	J	62/72 (86%)	37 (60%)	15 (24%)	10 (16%)	0	2
11	K	110/118 (93%)	83 (76%)	16 (14%)	11 (10%)	0	7
12	L	44/73 (60%)	20 (46%)	11 (25%)	13 (30%)	0	0
All	All	3759/4523 (83%)	2622 (70%)	748 (20%)	389 (10%)	0	6

All (389) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	48	PRO
1	A	54	ASN
1	A	57	LYS
1	A	67	CYS
1	A	73	GLY
1	A	74	MET
1	A	93	ILE
1	A	198	PRO
1	A	254	ASP
1	A	258	GLN
1	A	284	GLY
1	A	287	GLN
1	A	303	THR
1	A	304	TYR
1	A	312	GLN
1	A	313	PRO
1	A	336	ARG
1	A	365	VAL
1	A	383	GLN
1	A	411	GLY
1	A	425	ILE

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Mol	Chain	Res	Type
1	A	466	TYR
1	A	526	GLN
1	A	568	LYS
1	A	598	LEU
1	A	599	LEU
1	A	776	ILE
1	A	809	LEU
1	A	1015	ASN
1	A	1018	SER
1	A	1038	ARG
1	A	1117	ALA
1	A	1125	GLU
1	A	1126	ILE
1	A	1167	GLU
1	A	1208	GLN
1	A	1233	ASP
1	A	1235	ALA
1	A	1258	GLU
1	A	1284	LYS
1	A	1327	SER
1	A	1344	ILE
1	A	1408	THR
1	A	1441	THR
2	B	45	SER
2	B	54	PRO
2	B	93	ASP
2	B	95	THR
2	B	197	ASN
2	B	220	ALA
2	B	274	ILE
2	B	325	PHE
2	B	326	ILE
2	B	358	THR
2	B	360	GLU
2	B	394	PHE
2	B	463	LYS
2	B	613	ARG
2	B	622	ASP
2	B	634	GLU
2	B	640	ASP
2	B	705	GLU
2	B	869	SER

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Mol	Chain	Res	Type
2	B	879	ARG
2	B	881	THR
2	B	884	ARG
2	B	907	GLY
2	B	976	ILE
2	B	1046	PRO
2	B	1097	HIS
2	B	1100	ASP
2	B	1131	GLY
2	B	1155	SER
2	B	1156	ASP
2	B	1167	GLY
2	B	1171	VAL
2	B	1175	LEU
2	B	1182	CYS
2	B	1223	VAL
3	C	4	GLU
3	C	139	ASP
3	C	161	LYS
3	C	237	SER
4	D	48	LEU
4	D	91	LYS
4	D	139	PRO
4	D	167	LYS
5	E	73	ASP
5	E	86	SER
5	E	87	VAL
5	E	105	SER
6	F	73	ALA
6	F	74	ILE
7	G	52	MET
7	G	118	ASN
7	G	123	PRO
7	G	154	VAL
8	H	60	ALA
8	H	82	LYS
8	H	107	ASP
8	H	139	LEU
9	I	20	LYS
9	I	50	THR
9	I	51	ASN
9	I	56	ALA

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Mol	Chain	Res	Type
9	I	107	LYS
10	J	2	ILE
10	J	41	LYS
10	J	63	ASN
11	K	43	ALA
12	L	37	ALA
12	L	41	SER
12	L	46	ASP
12	L	47	PRO
12	L	52	GLU
12	L	61	ALA
12	L	62	ARG
1	A	35	ILE
1	A	55	ASP
1	A	58	LEU
1	A	62	ASP
1	A	69	THR
1	A	71	GLY
1	A	76	GLU
1	A	319	SER
1	A	416	LEU
1	A	424	ASP
1	A	467	SER
1	A	518	ASN
1	A	629	GLY
1	A	673	ASP
1	A	700	HIS
1	A	717	GLY
1	A	847	GLU
1	A	853	TYR
1	A	974	HIS
1	A	1004	GLY
1	A	1006	ASN
1	A	1016	ALA
1	A	1124	ARG
1	A	1214	VAL
1	A	1223	SER
1	A	1264	LYS
1	A	1317	ALA
1	A	1424	CYS
2	B	55	ARG
2	B	102	GLN

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Mol	Chain	Res	Type
2	B	167	SER
2	B	177	GLU
2	B	210	ALA
2	B	250	TYR
2	B	251	GLY
2	B	255	LYS
2	B	287	GLY
2	B	297	GLU
2	B	406	LEU
2	B	459	TRP
2	B	460	GLY
2	B	510	THR
2	B	523	GLY
2	B	550	PHE
2	B	552	GLU
2	B	702	MET
2	B	706	ASP
2	B	792	MET
2	B	813	LYS
2	B	888	GLY
2	B	946	ASN
2	B	1006	ILE
2	B	1069	PHE
2	B	1075	GLY
2	B	1099	VAL
2	B	1126	GLY
2	B	1151	LEU
2	B	1176	LYS
2	B	1186	LYS
3	C	17	VAL
3	C	133	VAL
3	C	149	ASN
3	C	156	ARG
3	C	173	CYS
3	C	184	ASN
4	D	53	LEU
4	D	92	VAL
4	D	163	LEU
4	D	170	ASN
5	E	29	ILE
5	E	44	LYS
5	E	119	ALA

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Mol	Chain	Res	Type
5	E	120	ASN
5	E	129	ALA
5	E	137	SER
6	F	154	ASP
7	G	50	ASP
7	G	139	LYS
8	H	18	GLY
8	H	62	SER
8	H	81	PRO
8	H	89	ALA
9	I	11	ASN
9	I	57	GLY
9	I	106	CYS
10	J	6	ARG
10	J	14	VAL
11	K	7	PHE
11	K	14	ASP
11	K	15	ASP
11	K	44	ASN
11	K	49	GLU
11	K	59	VAL
11	K	80	GLY
12	L	44	LYS
12	L	55	HIS
12	L	57	VAL
12	L	58	ILE
1	A	65	PHE
1	A	109	ASN
1	A	131	PRO
1	A	154	VAL
1	A	197	GLN
1	A	264	THR
1	A	329	ARG
1	A	337	LEU
1	A	419	HIS
1	A	592	THR
1	A	610	ASP
1	A	772	GLU
1	A	777	ALA
1	A	872	ASP
1	A	886	THR
1	A	988	ILE

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Mol	Chain	Res	Type
1	A	1122	LEU
1	A	1226	LEU
1	A	1269	HIS
1	A	1283	SER
1	A	1368	TYR
1	A	1389	ARG
2	B	17	CYS
2	B	42	MET
2	B	173	ARG
2	B	253	GLU
2	B	300	TRP
2	B	324	ASP
2	B	443	SER
2	B	453	SER
2	B	467	SER
2	B	524	GLN
2	B	584	ARG
2	B	635	ASP
2	B	848	ARG
2	B	883	LEU
2	B	909	ASP
2	B	951	GLN
2	B	1022	THR
2	B	1108	ARG
2	B	1121	GLY
2	B	1150	ARG
2	B	1158	PHE
2	B	1178	ASN
2	B	1181	GLU
3	C	89	ASP
3	C	132	PRO
3	C	148	ARG
4	D	54	SER
4	D	95	GLY
4	D	177	GLU
5	E	2	GLU
5	E	40	GLU
5	E	50	GLY
5	E	72	SER
6	F	81	THR
6	F	150	GLU
7	G	35	GLU

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Mol	Chain	Res	Type
7	G	94	VAL
7	G	165	GLU
7	G	167	PHE
8	H	80	PRO
8	H	108	GLU
9	I	47	GLU
10	J	24	LEU
12	L	45	SER
12	L	51	LYS
1	A	44	SER
1	A	45	ARG
1	A	196	ALA
1	A	318	LYS
1	A	323	VAL
1	A	535	MET
1	A	569	PRO
1	A	601	PRO
1	A	667	ILE
1	A	848	ASP
1	A	1116	PRO
1	A	1169	PHE
1	A	1338	ILE
1	A	1369	ARG
1	A	1406	GLU
2	B	33	GLN
2	B	43	GLU
2	B	101	PRO
2	B	382	ALA
2	B	568	THR
2	B	603	SER
2	B	724	LYS
2	B	842	ASN
2	B	1116	ARG
2	B	1136	ASP
3	C	106	GLY
3	C	153	LEU
3	C	169	LYS
4	D	142	ILE
5	E	191	ARG
7	G	67	SER
8	H	127	GLY
9	I	8	LEU

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Mol	Chain	Res	Type
9	I	9	GLU
9	I	34	TYR
9	I	86	PHE
11	K	54	PRO
11	K	78	GLU
11	K	111	ILE
1	A	234	TRP
1	A	311	GLY
1	A	651	GLN
1	A	707	PRO
1	A	753	LYS
1	A	960	VAL
1	A	981	SER
1	A	1013	GLN
1	A	1064	GLU
1	A	1206	ASP
1	A	1414	GLU
2	B	32	SER
2	B	175	LEU
2	B	254	ASP
2	B	296	ASP
2	B	429	ILE
2	B	462	GLN
2	B	587	SER
2	B	738	PHE
2	B	785	TYR
2	B	1177	LYS
2	B	1183	ARG
3	C	33	ARG
3	C	214	LYS
3	C	227	ARG
3	C	240	ALA
5	E	37	SER
5	E	85	PRO
5	E	202	GLU
6	F	106	PRO
6	F	151	LEU
7	G	17	TYR
8	H	12	VAL
8	H	91	ASP
8	H	118	GLY
10	J	43	TYR

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Mol	Chain	Res	Type
1	A	255	GLU
1	A	333	LYS
1	A	652	LYS
1	A	1017	THR
1	A	1401	MET
2	B	473	SER
2	B	1017	ILE
3	C	59	ASP
3	C	129	VAL
3	C	142	ILE
4	D	183	ASP
7	G	128	PRO
8	H	94	TYR
9	I	33	ASP
10	J	32	GLY
6	F	111	ILE
10	J	28	GLY
2	B	282	GLY
6	F	109	VAL
10	J	56	ILE
1	A	757	ILE
1	A	1244	VAL
2	B	457	GLY
4	D	161	PRO
1	A	245	PRO
1	A	378	PRO
2	B	543	PRO
2	B	977	GLY
2	B	992	VAL
2	B	629	PRO
6	F	105	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	988/1528 (65%)	875 (89%)	113 (11%)	5 20
2	B	822/1077 (76%)	724 (88%)	98 (12%)	5 19
3	C	155/264 (59%)	131 (84%)	24 (16%)	2 13
4	D	78/160 (49%)	64 (82%)	14 (18%)	2 11
5	E	155/197 (79%)	140 (90%)	15 (10%)	8 25
6	F	60/137 (44%)	53 (88%)	7 (12%)	5 19
7	G	102/148 (69%)	85 (83%)	17 (17%)	2 12
8	H	91/130 (70%)	82 (90%)	9 (10%)	7 24
9	I	82/109 (75%)	74 (90%)	8 (10%)	7 25
10	J	48/66 (73%)	39 (81%)	9 (19%)	1 9
11	K	67/109 (62%)	56 (84%)	11 (16%)	2 12
12	L	26/58 (45%)	24 (92%)	2 (8%)	12 33
All	All	2674/3983 (67%)	2347 (88%)	327 (12%)	5 19

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	18	GLN
1	A	34	LYS
1	A	41	MET
1	A	62	ASP
1	A	110	CYS
1	A	120	PRO
1	A	121	THR
1	A	131	PRO
1	A	154	VAL
1	A	158	SER
1	A	185	THR
1	A	198	PRO
1	A	200	ARG
1	A	216	SER
1	A	217	PRO
1	A	239	VAL
1	A	244	PRO
1	A	262	ASP

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Mol	Chain	Res	Type
1	A	271	LEU
1	A	290	ILE
1	A	303	THR
1	A	309	ILE
1	A	313	PRO
1	A	336	ARG
1	A	345	ARG
1	A	370	SER
1	A	386	ILE
1	A	390	THR
1	A	404	LYS
1	A	406	VAL
1	A	409	ASP
1	A	413	ARG
1	A	426	VAL
1	A	441	ASP
1	A	444	LEU
1	A	446	ASN
1	A	448	GLN
1	A	451	LEU
1	A	452	HIS
1	A	462	LYS
1	A	463	VAL
1	A	467	SER
1	A	470	ARG
1	A	494	GLN
1	A	498	THR
1	A	506	CYS
1	A	521	VAL
1	A	525	VAL
1	A	543	GLU
1	A	561	VAL
1	A	592	THR
1	A	598	LEU
1	A	617	VAL
1	A	636	ARG
1	A	651	GLN
1	A	667	ILE
1	A	671	ILE
1	A	677	MET
1	A	691	VAL
1	A	707	PRO

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Mol	Chain	Res	Type
1	A	719	VAL
1	A	722	THR
1	A	728	ASP
1	A	739	LYS
1	A	741	LEU
1	A	775	ARG
1	A	789	THR
1	A	822	ARG
1	A	859	ASN
1	A	883	THR
1	A	887	ILE
1	A	924	VAL
1	A	927	GLN
1	A	930	LEU
1	A	941	ARG
1	A	986	PRO
1	A	1031	ARG
1	A	1050	THR
1	A	1052	GLU
1	A	1054	GLN
1	A	1118	LEU
1	A	1122	LEU
1	A	1135	VAL
1	A	1148	VAL
1	A	1154	ILE
1	A	1161	THR
1	A	1168	ASP
1	A	1196	ARG
1	A	1238	LEU
1	A	1244	VAL
1	A	1258	GLU
1	A	1267	GLU
1	A	1270	MET
1	A	1274	ILE
1	A	1280	PRO
1	A	1288	VAL
1	A	1294	VAL
1	A	1300	GLU
1	A	1327	SER
1	A	1335	PHE
1	A	1371	MET
1	A	1374	LEU

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Mol	Chain	Res	Type
1	A	1388	THR
1	A	1403	CYS
1	A	1406	GLU
1	A	1427	VAL
1	A	1429	GLU
1	A	1435	GLN
1	A	1444	PHE
1	A	1447	MET
1	A	1448	ILE
1	A	1450	GLU
2	B	17	CYS
2	B	50	VAL
2	B	54	PRO
2	B	87	PRO
2	B	88	THR
2	B	90	THR
2	B	115	VAL
2	B	166	ARG
2	B	174	THR
2	B	178	VAL
2	B	185	GLU
2	B	208	ARG
2	B	216	VAL
2	B	226	SER
2	B	252	ARG
2	B	259	ARG
2	B	260	THR
2	B	290	LEU
2	B	295	TYR
2	B	358	THR
2	B	364	GLU
2	B	365	THR
2	B	386	LYS
2	B	416	LYS
2	B	441	VAL
2	B	444	THR
2	B	458	ASN
2	B	459	TRP
2	B	469	ARG
2	B	475	VAL
2	B	478	ARG
2	B	489	ARG

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Mol	Chain	Res	Type
2	B	491	THR
2	B	506	GLN
2	B	509	ASN
2	B	543	PRO
2	B	544	SER
2	B	568	THR
2	B	575	VAL
2	B	584	ARG
2	B	596	LEU
2	B	602	ILE
2	B	603	SER
2	B	607	SER
2	B	609	ILE
2	B	621	THR
2	B	622	ASP
2	B	628	ARG
2	B	637	GLU
2	B	648	THR
2	B	676	TYR
2	B	686	VAL
2	B	703	THR
2	B	722	THR
2	B	737	THR
2	B	755	ILE
2	B	787	VAL
2	B	790	ASP
2	B	791	THR
2	B	797	TYR
2	B	798	TYR
2	B	811	TYR
2	B	831	SER
2	B	835	GLN
2	B	839	MET
2	B	845	SER
2	B	859	TYR
2	B	881	THR
2	B	887	HIS
2	B	899	ILE
2	B	939	THR
2	B	944	THR
2	B	953	LEU
2	B	970	THR

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Mol	Chain	Res	Type
2	B	986	GLN
2	B	997	GLU
2	B	999	MET
2	B	1021	MET
2	B	1022	THR
2	B	1045	THR
2	B	1046	PRO
2	B	1047	PHE
2	B	1069	PHE
2	B	1071	VAL
2	B	1084	GLN
2	B	1092	TYR
2	B	1095	LEU
2	B	1096	ARG
2	B	1103	ILE
2	B	1147	LEU
2	B	1151	LEU
2	B	1159	ARG
2	B	1185	CYS
2	B	1189	THR
2	B	1202	LEU
2	B	1211	ASN
2	B	1218	THR
2	B	1224	SER
3	C	9	ILE
3	C	34	ARG
3	C	66	LEU
3	C	76	VAL
3	C	86	THR
3	C	96	VAL
3	C	101	SER
3	C	111	THR
3	C	121	VAL
3	C	124	PRO
3	C	136	ASP
3	C	147	LEU
3	C	163	ILE
3	C	166	GLU
3	C	194	GLU
3	C	195	VAL
3	C	208	THR
3	C	215	PRO

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Mol	Chain	Res	Type
3	C	231	THR
3	C	233	GLU
3	C	234	THR
3	C	235	THR
3	C	251	LEU
3	C	262	LEU
4	D	30	LEU
4	D	32	PRO
4	D	41	HIS
4	D	48	LEU
4	D	51	LEU
4	D	109	LEU
4	D	111	THR
4	D	117	ASP
4	D	139	PRO
4	D	158	THR
4	D	169	VAL
4	D	171	LEU
4	D	184	PRO
4	D	185	TYR
5	E	8	ILE
5	E	16	ARG
5	E	29	ILE
5	E	32	GLU
5	E	37	SER
5	E	59	PHE
5	E	65	PRO
5	E	72	SER
5	E	73	ASP
5	E	77	LEU
5	E	103	ASN
5	E	113	ASN
5	E	131	ILE
5	E	143	ILE
5	E	174	LEU
6	F	74	ILE
6	F	90	ARG
6	F	99	LEU
6	F	103	MET
6	F	116	ASP
6	F	133	VAL
6	F	138	LEU

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Mol	Chain	Res	Type
7	G	1	MET
7	G	13	LEU
7	G	32	THR
7	G	37	THR
7	G	46	VAL
7	G	49	LEU
7	G	74	TYR
7	G	77	VAL
7	G	80	LYS
7	G	88	ASP
7	G	111	SER
7	G	112	THR
7	G	128	PRO
7	G	150	THR
7	G	154	VAL
7	G	163	ILE
7	G	171	ILE
8	H	3	SER
8	H	10	PHE
8	H	42	ILE
8	H	56	THR
8	H	63	LEU
8	H	95	VAL
8	H	101	TYR
8	H	102	LYS
8	H	109	ASP
9	I	12	ASN
9	I	14	LEU
9	I	15	TYR
9	I	50	THR
9	I	51	ASN
9	I	87	GLN
9	I	98	THR
9	I	100	PHE
10	J	2	ILE
10	J	7	CYS
10	J	13	VAL
10	J	16	ASP
10	J	22	LEU
10	J	42	ARG
10	J	43	TYR
10	J	45	CYS

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Mol	Chain	Res	Type
10	J	63	ASN
11	K	1	MET
11	K	10	PHE
11	K	16	VAL
11	K	17	PRO
11	K	25	SER
11	K	47	ARG
11	K	54	PRO
11	K	57	THR
11	K	76	GLN
11	K	94	ILE
11	K	101	LEU
12	L	29	VAL
12	L	65	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	68	GLN
1	A	172	GLN
1	A	226	ASN
1	A	274	ASN
1	A	300	HIS
1	A	340	ASN
1	A	436	HIS
1	A	480	ASN
1	A	491	HIS
1	A	494	GLN
1	A	504	GLN
1	A	699	GLN
1	A	737	ASN
1	A	742	ASN
1	A	743	ASN
1	A	746	GLN
1	A	758	ASN
1	A	787	HIS
1	A	859	ASN
1	A	882	GLN
1	A	955	ASN
1	A	968	ASN
1	A	1084	ASN

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Mol	Chain	Res	Type
1	A	1213	GLN
1	A	1234	ASN
1	A	1367	ASN
1	A	1390	HIS
1	A	1393	ASN
2	B	108	ASN
2	B	206	GLN
2	B	227	HIS
2	B	350	GLN
2	B	356	HIS
2	B	359	GLN
2	B	426	GLN
2	B	458	ASN
2	B	508	HIS
2	B	509	ASN
2	B	531	ASN
2	B	583	HIS
2	B	651	HIS
2	B	708	GLN
2	B	744	HIS
2	B	767	ASN
2	B	821	GLN
2	B	822	ASN
2	B	835	GLN
2	B	842	ASN
2	B	975	GLN
2	B	1015	HIS
2	B	1065	GLN
2	B	1084	GLN
2	B	1141	HIS
2	B	1161	HIS
2	B	1179	GLN
2	B	1195	HIS
3	C	167	HIS
3	C	184	ASN
3	C	252	GLN
4	D	144	GLN
5	E	31	GLN
5	E	100	GLN
5	E	103	ASN
5	E	113	ASN
5	E	142	ASN

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Mol	Chain	Res	Type
5	E	146	HIS
7	G	53	ASN
8	H	136	GLN
9	I	79	HIS
11	K	65	HIS
11	K	76	GLN
11	K	110	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	1409/1743 (80%)	-0.04	26 (1%) 67 53	110, 206, 318, 455	0
2	B	1079/1227 (87%)	-0.01	15 (1%) 73 58	115, 226, 316, 418	0
3	C	263/304 (86%)	0.04	2 (0%) 82 68	148, 216, 311, 349	0
4	D	143/186 (76%)	0.11	4 (2%) 55 42	167, 263, 321, 343	0
5	E	214/214 (100%)	-0.03	3 (1%) 73 58	122, 197, 260, 300	0
6	F	84/155 (54%)	-0.04	2 (2%) 59 47	160, 222, 270, 312	0
7	G	171/171 (100%)	0.14	4 (2%) 61 48	156, 213, 267, 311	0
8	H	131/145 (90%)	0.13	4 (3%) 51 40	161, 214, 298, 344	0
9	I	113/115 (98%)	0.08	4 (3%) 47 37	211, 276, 343, 386	0
10	J	64/72 (88%)	0.05	1 (1%) 70 55	154, 214, 272, 288	0
11	K	112/118 (94%)	-0.03	2 (1%) 67 53	149, 202, 274, 293	0
12	L	46/73 (63%)	-0.01	0 100 100	223, 275, 329, 350	0
All	All	3829/4523 (84%)	-0.00	67 (1%) 69 54	110, 219, 314, 455	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	115	LEU	4.0
8	H	118	GLY	3.9
4	D	32	PRO	3.7
7	G	42	PHE	3.5
2	B	1191	ILE	3.4
3	C	230	MET	3.3
7	G	36	GLY	3.2
2	B	522	GLU	3.1
4	D	181	LEU	3.1
2	B	634	GLU	3.1
1	A	1272	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1304	GLU	3.0
6	F	148	CYS	2.9
1	A	909	ILE	2.8
1	A	93	ILE	2.8
1	A	613	VAL	2.8
4	D	129	HIS	2.8
1	A	406	VAL	2.7
1	A	880	GLU	2.6
1	A	1224	ASP	2.6
6	F	93	ILE	2.5
7	G	41	GLN	2.5
8	H	77	SER	2.5
2	B	327	GLY	2.5
1	A	1257	ALA	2.5
1	A	838	ILE	2.4
11	K	102	ASP	2.4
1	A	542	ILE	2.4
1	A	96	ILE	2.4
1	A	1271	LEU	2.3
11	K	42	LEU	2.3
1	A	1381	ARG	2.3
2	B	439	LEU	2.3
5	E	166	ARG	2.3
8	H	26	ILE	2.3
9	I	62	ILE	2.3
1	A	314	GLN	2.3
2	B	408	ASN	2.3
1	A	496	GLU	2.2
9	I	63	GLY	2.2
2	B	685	GLY	2.2
1	A	506	CYS	2.2
4	D	161	PRO	2.2
5	E	208	ALA	2.2
2	B	568	THR	2.2
1	A	1190	GLN	2.2
1	A	802	GLU	2.2
9	I	18	GLU	2.2
2	B	728	PRO	2.2
1	A	179	GLY	2.1
10	J	64	PRO	2.1
2	B	532	LEU	2.1
1	A	502	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	424	ASP	2.1
2	B	753	ALA	2.1
7	G	138	THR	2.1
2	B	895	GLU	2.1
2	B	896	ASP	2.0
1	A	1036	GLU	2.0
2	B	775	LYS	2.0
5	E	163	LEU	2.0
1	A	814	PHE	2.0
2	B	297	GLU	2.0
3	C	178	PHE	2.0
9	I	53	GLY	2.0
8	H	38	LEU	2.0
1	A	1219	SER	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	A	1801	1/1	0.94	0.06	299,299,299,299	0
13	ZN	A	1802	1/1	0.95	0.06	270,270,270,270	0
13	ZN	C	401	1/1	0.95	0.06	283,283,283,283	0
13	ZN	I	201	1/1	0.96	0.05	239,239,239,239	0
13	ZN	L	101	1/1	0.97	0.06	318,318,318,318	0
13	ZN	J	101	1/1	0.98	0.07	158,158,158,158	0
13	ZN	I	202	1/1	0.98	0.05	242,242,242,242	0
13	ZN	B	1301	1/1	0.99	0.03	248,248,248,248	0

6.5 Other polymers [i](#)

There are no such residues in this entry.