



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2017 – 01:50 PM EDT

PDB ID : 5D4W  
Title : Crystal structure of Hsp104  
Authors : Heuck, A.; Schitter-Sollner, S.; Clausen, T.  
Deposited on : unknown  
Resolution : 3.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

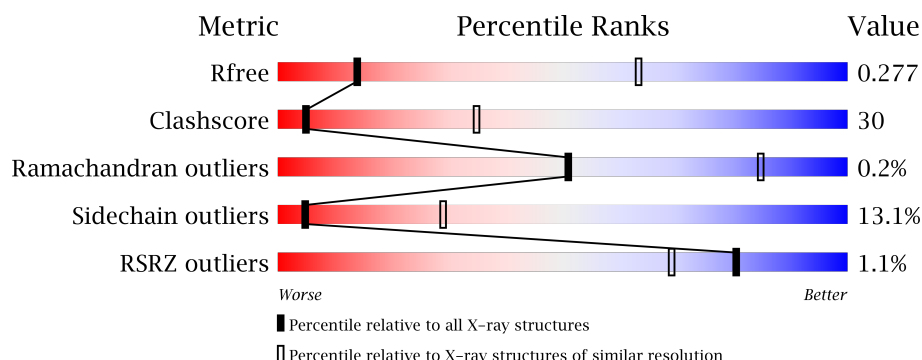
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1234 (3.90-3.50)
Clashscore	112137	1377 (3.90-3.50)
Ramachandran outliers	110173	1323 (3.90-3.50)
Sidechain outliers	110143	1320 (3.90-3.50)
RSRZ outliers	101464	1262 (3.90-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	926	<div> <div></div> <div> <div></div> <div>33%</div> <div>35%</div> <div>6%</div> <div>26%</div> </div> </div>
1	B	926	<div> <div></div> <div> <div></div> <div>32%</div> <div>37%</div> <div>6%</div> <div>26%</div> </div> </div>
1	C	926	<div> <div></div> <div> <div></div> <div>34%</div> <div>34%</div> <div>6%</div> <div>26%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	A	1001	-	-	X	-
2	ADP	B	1001	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16269 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 Putative heat shock protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	688	Total	C	N	O	S	Se	0	0	0
			5369	3354	985	1009	5	16			
1	B	688	Total	C	N	O	S	Se	0	0	0
			5369	3354	985	1009	5	16			
1	C	688	Total	C	N	O	S	Se	0	0	0
			5369	3354	985	1009	5	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP G0S4G4
A	296	ALA	GLU	engineered mutation	UNP G0S4G4
A	707	ALA	GLU	engineered mutation	UNP G0S4G4
B	1	MSE	-	initiating methionine	UNP G0S4G4
B	296	ALA	GLU	engineered mutation	UNP G0S4G4
B	707	ALA	GLU	engineered mutation	UNP G0S4G4
C	1	MSE	-	initiating methionine	UNP G0S4G4
C	296	ALA	GLU	engineered mutation	UNP G0S4G4
C	707	ALA	GLU	engineered mutation	UNP G0S4G4

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

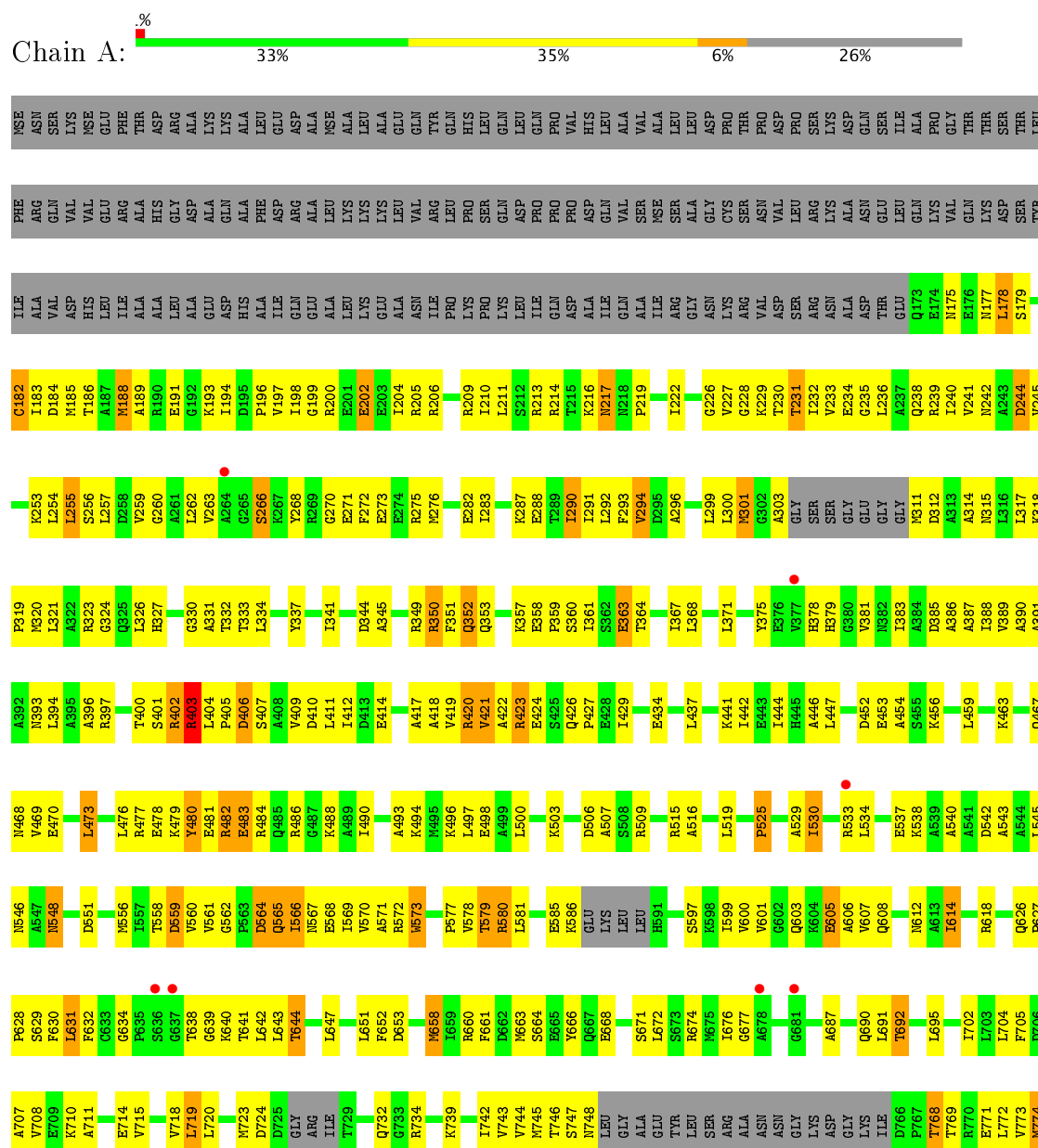


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	C	1	Total 27	C 10	N 5	O 10	P 2	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Putative heat shock protein





- Molecule 1: Putative heat shock protein



IE	VAL	ASP	HIS	LEU	IE	ALA	LEU	ALA	GLU	ASP	HIS	LEU	LYS	GLU	ASN	IE	PRO	PRO	LYS	LEU	GLN	GLY	ASP	ALA	ALA	GLN	ALA	IE	IE	IE	IE	ARG	ARG	GLY	ASN	LYS	ARG	VAL	VAL	ASP	SER	ASP	ASN	ALA	ASP	THR	GLU	Q173	E176	M177	L178	S179	K180	E181	L182	M183	L184	K185	E186	L187	M188	L189	K190	E191	L192	M193	L194	K195	E196	L197	M198	L199	K200	E201	L202	M203	L204	K205	E206	L207	M208	L209	K210	E211	L212	M213	L214	K215	E216	L217	M218	L219	K220	E221	L222	M223	L224	K225	E226	L227	M228	L229	K230	E231	L232	M233	L234	K235	E236	L237	M238	L239	K240	E241	L242	M243	L244	K245	E246	L247	M248	L249	K250	E251	L252	M253	L254	K255	E256	L257	M258	L259	K260	E261	L262	M263	L264	K265	E266	L267	M268	L269	K270	E271	L272	M273	L274	K275	E276	L277	M278	L279	K280	E281	L282	M283	L284	K285	E286	L287	M288	L289	K290	E291	L292	M293	L294	K295	E296	L297	M298	L299	K300	E301	L302	M303	L304	K305	E306	L307	M308	L309	K310	E311	L312	M313	L314	K315	E316	L317	M318	L319	K320	E321	L322	M323	L324	K325	E326	L327	M328	L329	K330	E331	L332	M333	L334	K335	E336	L337	M338	L339	K340	E341	L342	M343	L344	K345	E346	L347	M348	L349	K350	E351	L352	M353	L354	K355	E356	L357	M358	L359	K360	E361	L362	M363	L364	K365	E366	L367	M368	L369	K370	E371	L372	M373	L374	K375	E376	L377	M378	L379	K380	E381	L382	M383	L384	K385	E386	L387	M388	L389	K390	E391	L392	M393	L394	K395	E396	L397	M398	L399	K400	E401	L402	M403	L404	K405	E406	L407	M408	L409	K410	E411	L412	M413	L414	K415	E416	L417	M418	L419	K420	E421	L422	M423	L424	K425	E426	L427	M428	L429	K430	E431	L432	M433	L434	K435	E436	L437	M438	L439	K440	E441	L442	M443	L444	K445	E446	L447	M448	L449	K450	E451	L452	M453	L454	K455	E456	L457	M458	L459	K460	E461	L462	M463	L464	K465	E466	L467	M468	L469	K470	E471	L472	M473	L474	K475	E476	L477	M478	L479	K480	E481	L482	M483	L484	K485	E486	L487	M488	L489	K490	E491	L492	M493	L494	K495	E496	L497	M498	L499	K500	E501	L502	M503	L504	K505	E506	L507	M508	L509	K510	E511	L512	M513	L514	K515	E516	L517	M518	L519	K520	E521	L522	M523	L524	K525	E526	L527	M528	L529	K530	E531	L532	M533	L534	K535	E536	L537	M538	L539	K540	E541	L542	M543	L544	K545	E546	L547	M548	L549	K550	E551	L552	M553	L554	K555	E556	L557	M558	L559	K560	E561	L562	M563	L564	K565	E566	L567	M568	L569	K570	E571	L572	M573	L574	K575	E576	L577	M578	L579	K580	E581	L582	M583	L584	K585	E586	L587	M588	L589	K590	E591	L592	M593	L594	K595	E596	L597	M598	L599	K600	E601	L602	M603	L604	K605	E606	L607	M608	L609	K610	E611	L612	M613	L614	K615	E616	L617	M618	L619	K620	E621	L622	M623	L624	K625	E626	L627	M628	L629	K630	E631	L632	M633	L634	K635	E636	L637	M638	L639	K640	E641	L642	M643	L644	K645	E646	L647	M648	L649	K650	E651	L652	M653	L654	K655	E656	L657	M658	L659	K660	E661	L662	M663	L664	K665	E666	L667	M668	L669	K670	E671	L672	M673	L674	K675	E676	L677	M678	L679	K680	E681	L682	M683	L684	K685	E686	L687	M688	L689	K690	E691	L692	M693	L694	K695	E696	L697	M698	L699	K700	E701	L702	M703	L704	K705	E706	L707	M708	L709	K710	E711	L712	M713	L714	K715	E716	L717	M718	L719	K720	E721	L722	M723	L724	K725	E726	L727	M728	L729	K730	E731	L732	M733	L734	K735	E736	L737	M738	L739	K740	E741	L742	M743	L744	K745	E746	L747	M748	L749	K750	E751	L752	M753	L754	K755	E756	L757	M758	L759	K760	E761	L762	M763	L764	K765	E766	L767	M768	L769	K770	E771	L772	M773	L774	K775	E776	L777	M778	L779	K780	E781	L782	M783	L784	K785	E786	L787	M788	L789	K790	E791	L792	M793	L794	K795	E796	L797	M798	L799	K800	E801	L802	M803	L804	K805	E806	L807	M808	L809	K810	E811	L812	M813	L814	K815	E816	L817	M818	L819	K820	E821	L822	M823	L824	K825	E826	L827	M828	L829	K830	E831	L832	M833	L834	K835	E836	L837	M838	L839	K840	E841	L842	M843	L844	K845	E846	L847	M848	L849	K850	E851	L852	M853	L854	K855	E856	L857	M858	L859	K860	E861	L862	M863	L864	K865	E866	L867	M868	L869	K870	E871	L872	M873	L874	K875	E876	L877	M878	L879	K880	E881	L882	M883	L884	K885	E886	L887	M888	L889	K890	E891	L892	M893	L894	K895	E896	L897	M898	L899	K900	E901	L902	M903	L904	K905	E906	L907	M908	L909	K910	E911	L912	M913	L914	K915	E916	L917	M918	L919	K920	E921	L922	M923	L924	K925	E926	L927	M928	L929	K930	E931	L932	M933	L934	K935	E936	L937	M938	L939	K940	E941	L942	M943	L944	K945	E946	L947	M948	L949	K950	E951	L952	M953	L954	K955	E956	L957	M958	L959	K960	E961	L962	M963	L964	K965	E966	L967	M968	L969	K970	E971	L972	M973	L974	K975	E976	L977	M978	L979	K980	E981	L982	M983	L984	K985	E986	L987	M988	L989	K990	E991	L992	M993	L994	K995	E996	L997	M998	L999	K1000
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C182	I183	D184	M185	I186	A187	M188	G189	I190	I191	D192	M193	I194	D195	P196	P197	I198	G199	R200	R201	R202	R203	R204	R205	R206	R207	R208	R209	R210	L211	S212	R213	R214	R215	R216	R217	R218	P219	V220	L221	L222	G223	E224	P225	G226	V227	G228	R229	R230	R231	R232	R233	G234	G235	L236	A237	R238	R239	L240	V241	N242	A243	D244	D245	P246
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■ A250 ■ K263 ■ L264 ■ L265 ■ S266 ■ L267 ■ L262 ■ G270 ■ E271 ■ F272 ■ E273 ■ E274 ■ R275 ■ L276 ■ L280 ■ L281 ■ E282 ■ L283 ■ S286 ■ L287 ■ L290 ■ L291 ■ L292 ■ F293 ■ V294 ■ L299 ■ L300 ■ L301 ■ G302 ■ A303 ■ GLY ■ SER ■ SER ■ GLY ■ GLY ■ GLY ■ GLY ■ K311 ■ L312 ■ L313 ■ L314 ■ N315 ■ L316 ■ L317 ■ L318 ■ F319 ■ K320 ■ L321 ■ L326 ■ E327 ■ C328

<b>T329</b>	<b>G330</b>	<b>A331</b>	<b>T332</b>	<b>T333</b>	<b>Y337</b>	<b>R338</b>	<b>K339</b>	<b>Y340</b>	<b>I341</b>	<b>E342</b>	<b>K343</b>	<b>R344</b>	<b>A345</b>	<b>A346</b>	<b>F347</b>	<b>E348</b>	<b>R349</b>	<b>R350</b>	<b>F351</b>	<b>Q352</b>	<b>Q353</b>	<b>K357</b>	<b>E358</b>	<b>P359</b>	<b>S360</b>	<b>S361</b>	<b>S362</b>	<b>E363</b>	<b>T364</b>	<b>I365</b>	<b>I366</b>	<b>S366</b>	<b>I367</b>	<b>R368</b>	<b>R369</b>	<b>G370</b>	<b>L371</b>	<b>H379</b>	<b>V381</b>	<b>T382</b>	<b>T383</b>	<b>A386</b>	<b>R387</b>	<b>R388</b>	<b>P389</b>	<b>A390</b>	<b>Z391</b>	<b>A392</b>	<b>N393</b>	<b>L394</b>	<b>A395</b>	<b>A396</b>	<b>R397</b>	<b>T400</b>
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S401	R402	R403	R404	L404	R405	R406	S407	A408	V409	L412	A417	A418	V419	R420	V421	A422	R423	E424	S425	Q426	L430	L433	E434	R435	R436	L437	R438	K441	L442	E443	L444	L447	K456	A457	R458	L459	A460	Q461	A462	K463	Q464	Q467	N468	V469	R475	L476	R477	E478	K479	E480	V481	Y482	Y483	Y484	Y485	Y486	Y487	Y488	Y489	Y490	Y491	Y492	Y493	Y494	Y495	Y496	Y497	Y498	Y499	Y500	Y501	Y502	Y503	Y504	Y505	Y506	Y507	Y508	Y509	Y510	Y511	Y512	Y513	Y514	Y515	Y516	Y517	Y518	Y519	Y520	Y521	Y522	Y523	Y524	Y525	Y526	Y527	Y528	Y529	Y530	Y531	Y532	Y533	Y534	Y535	Y536	Y537	Y538	Y539	Y540	Y541	Y542	Y543	Y544	Y545	Y546	Y547	Y548	Y549	Y550	Y551	Y552	Y553	Y554	Y555	Y556	Y557	Y558	Y559	Y560	Y561	Y562	Y563	Y564	Y565	Y566	Y567	Y568	Y569	Y570	Y571	Y572	Y573	Y574	Y575	Y576	Y577	Y578	Y579	Y580	Y581	Y582	Y583	Y584	Y585	Y586	Y587	Y588	Y589	Y590	Y591	Y592	Y593	Y594	Y595	Y596	Y597	Y598	Y599	Y600	Y601	Y602	Y603	Y604	Y605	Y606	Y607	Y608	Y609	Y610	Y611	Y612	Y613	Y614	Y615	Y616	Y617	Y618	Y619	Y620	Y621	Y622	Y623	Y624	Y625	Y626	Y627	Y628	Y629	Y630	Y631	Y632	Y633	Y634	Y635	Y636	Y637	Y638	Y639	Y640	Y641	Y642	Y643	Y644	Y645	Y646	Y647	Y648	Y649	Y650	Y651	Y652	Y653	Y654	Y655	Y656	Y657	Y658	Y659	Y660	Y661	Y662	Y663	Y664	Y665	Y666	Y667	Y668	Y669	Y670	Y671	Y672	Y673	Y674	Y675	Y676	Y677	Y678	Y679	Y680	Y681	Y682	Y683	Y684	Y685	Y686	Y687	Y688	Y689	Y690	Y691	Y692	Y693	Y694	Y695	Y696	Y697	Y698	Y699	Y700	Y701	Y702	Y703	Y704	Y705	Y706	Y707	Y708	Y709	Y710	Y711	Y712	Y713	Y714	Y715	Y716	Y717	Y718	Y719	Y720	Y721	Y722	Y723	Y724	Y725	Y726	Y727	Y728	Y729	Y730	Y731	Y732	Y733	Y734	Y735	Y736	Y737	Y738	Y739	Y740	Y741	Y742	Y743	Y744	Y745	Y746	Y747	Y748	Y749	Y750	Y751	Y752	Y753	Y754	Y755	Y756	Y757	Y758	Y759	Y760	Y761	Y762	Y763	Y764	Y765	Y766	Y767	Y768	Y769	Y770	Y771	Y772	Y773	Y774	Y775	Y776	Y777	Y778	Y779	Y780	Y781	Y782	Y783	Y784	Y785	Y786	Y787	Y788	Y789	Y790	Y791	Y792	Y793	Y794	Y795	Y796	Y797	Y798	Y799	Y800	Y801	Y802	Y803	Y804	Y805	Y806	Y807	Y808	Y809	Y810	Y811	Y812	Y813	Y814	Y815	Y816	Y817	Y818	Y819	Y820	Y821	Y822	Y823	Y824	Y825	Y826	Y827	Y828	Y829	Y830	Y831	Y832	Y833	Y834	Y835	Y836	Y837	Y838	Y839	Y840	Y841	Y842	Y843	Y844	Y845	Y846	Y847	Y848	Y849	Y850	Y851	Y852	Y853	Y854	Y855	Y856	Y857	Y858	Y859	Y860	Y861	Y862	Y863	Y864	Y865	Y866	Y867	Y868	Y869	Y870	Y871	Y872	Y873	Y874	Y875	Y876	Y877	Y878	Y879	Y880	Y881	Y882	Y883	Y884	Y885	Y886	Y887	Y888	Y889	Y890	Y891	Y892	Y893	Y894	Y895	Y896	Y897	Y898	Y899	Y900	Y901	Y902	Y903	Y904	Y905	Y906	Y907	Y908	Y909	Y910	Y911	Y912	Y913	Y914	Y915	Y916	Y917	Y918	Y919	Y920	Y921	Y922	Y923	Y924	Y925	Y926	Y927	Y928	Y929	Y930	Y931	Y932	Y933	Y934	Y935	Y936	Y937	Y938	Y939	Y940	Y941	Y942	Y943	Y944	Y945	Y946	Y947	Y948	Y949	Y950	Y951	Y952	Y953	Y954	Y955	Y956	Y957	Y958	Y959	Y960	Y961	Y962	Y963	Y964	Y965	Y966	Y967	Y968	Y969	Y970	Y971	Y972	Y973	Y974	Y975	Y976	Y977	Y978	Y979	Y980	Y981	Y982	Y983	Y984	Y985	Y986	Y987	Y988	Y989	Y990	Y991	Y992	Y993	Y994	Y995	Y996	Y997	Y998	Y999	Y1000
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784	785	786	787	788	789	790	791	792	793	794	795	796	797	798	799	800	801	802	803	804	805	806	807	808	809	810	811	812	813	814	815	816	817	818	819	820	821	822	823	824	825	826	827	828	829	830	831	832	833	834	835	836	837	838	839	840	841	842	843	844	845	846	847	848	849	850	851	852	853	854	855	856	857	858	859	860	861	862	863	864	865	866	867	868	869	870	871	872	873	874	875	876	877	878	879	880	881	882	883	884	885	886	887	888	889	890	891	892	893	894	895	896	897	898	899	900	901	902	903	904	905	906	907	908	909	910	911	912	913	914	915	916	917	918	919	920	921	922	923	924	925	926	927	928	929	930	931	932	933	934	935	936	937	938	939	940	941	942	943	944	945	946	947	948	949	950	951	952	953	954	955	956	957	958	959	960	961	962	963	964	965	966	967	968	969	970	971	972	973	974	975	976	977	978	979	980	981	982	983	984	985	986	987	988	989	990	991	992	993	994	995	996	997	998	999	1000
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.92Å 93.17Å 144.42Å 90.00° 119.72° 90.00°	Depositor
Resolution (Å)	47.58 – 3.70 47.58 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.58-3.70) 97.0 (47.58-3.60)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 3.57Å)	Xtriage
Refinement program	PHENIX (dev_2356: ???)	Depositor
R, $R_{free}$	0.237 , 0.277 0.237 , 0.277	Depositor DCC
$R_{free}$ test set	1778 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	116.6	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 239.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.259 for l,k,-h-l 0.259 for -h-l,k,h 0.167 for -h-l,-k,l 0.157 for h,-k,-h-l 0.166 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16269	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	210.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

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

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

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	0.31	0/5414	0.54	2/7262 (0.0%)
1	B	0.38	0/5414	0.61	3/7262 (0.0%)
1	C	0.32	0/5414	0.55	1/7262 (0.0%)
All	All	0.34	0/16242	0.57	6/21786 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	1
All	All	0	6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	653	ASP	C-N-CA	-6.95	104.33	121.70
1	B	368	LEU	CA-CB-CG	6.87	131.10	115.30
1	B	653	ASP	C-N-CA	-6.72	104.90	121.70
1	B	195	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	653	ASP	C-N-CA	-5.50	107.96	121.70
1	A	447	LEU	CA-CB-CG	5.22	127.32	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	SER	Peptide
1	A	402	ARG	Peptide
1	B	243	ALA	Peptide
1	B	385	ASP	Peptide
1	B	402	ARG	Peptide
1	C	402	ARG	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	5369	0	5537	323	0
1	B	5369	0	5537	397	0
1	C	5369	0	5537	331	0
2	A	54	0	24	11	0
2	B	54	0	24	18	0
2	C	54	0	24	4	0
All	All	16269	0	16683	994	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 30.

All (994) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LYS:HB3	1:C:352:GLN:HB3	1.46	0.97
1:A:216:LYS:HB3	1:A:352:GLN:HB3	1.46	0.97
1:B:562:GLY:H	1:B:565:GLN:HB2	1.29	0.96
1:B:379:HIS:HA	1:B:420:ARG:HH12	1.31	0.91
1:B:200:ARG:HG3	1:B:232:ILE:HD11	1.55	0.89
1:A:836:LYS:HD3	1:A:886:LYS:HE2	1.56	0.88
1:C:618:ARG:HG3	1:C:651:LEU:HD11	1.56	0.86
1:B:200:ARG:HG2	2:B:1001:ADP:HN61	1.36	0.85
1:C:397:ARG:HH12	1:C:652:PHE:HA	1.44	0.82
1:B:836:LYS:HD3	1:B:886:LYS:HE2	1.59	0.82
1:B:524:ILE:HG12	1:B:525:PRO:HD3	1.63	0.81
1:A:628:PRO:HB2	1:A:742:ILE:HG13	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:HB2	1:A:292:LEU:HD11	1.63	0.81
1:B:634:GLY:HA3	1:B:795:PHE:HB2	1.64	0.80
1:A:185:MSE:HE1	1:A:194:ILE:HG13	1.63	0.80
1:C:571:ALA:HB2	1:C:578:VAL:HG13	1.62	0.80
1:A:603:GLN:HB3	1:A:606:ALA:HB3	1.64	0.80
1:A:493:ALA:HB1	1:A:530:ILE:HG13	1.64	0.79
1:B:568:GLU:O	1:B:572:ARG:N	2.10	0.79
1:A:182:CYS:HB2	1:A:257:LEU:HA	1.65	0.79
1:B:227:VAL:O	2:B:1001:ADP:H8	1.65	0.78
1:B:829:VAL:HG12	1:B:880:VAL:HB	1.63	0.78
1:B:240:ILE:HG12	1:B:245:VAL:HB	1.64	0.78
1:B:396:ALA:O	1:B:400:THR:OG1	2.01	0.77
1:C:614:ILE:HD11	1:C:651:LEU:HD22	1.67	0.77
1:A:663:MSE:HB2	1:A:707:ALA:HB3	1.66	0.77
1:B:611:SER:OG	1:B:615:ARG:NH2	2.16	0.77
1:C:640:LYS:NZ	1:C:747:SER:O	2.16	0.77
1:C:490:ILE:HD11	1:C:533:ARG:HB2	1.66	0.77
1:A:364:THR:HG21	1:A:404:LEU:HB3	1.65	0.76
1:B:814:ILE:HG13	1:B:817:ARG:HE	1.50	0.76
1:A:543:ALA:HA	1:A:546:ASN:HB3	1.67	0.76
1:C:578:VAL:HG12	1:C:581:LEU:HD22	1.65	0.76
1:A:427:PRO:HG3	1:A:556:MSE:HG3	1.67	0.76
1:B:293:PHE:CE2	1:B:331:ALA:HB2	2.20	0.76
1:A:814:ILE:HG13	1:A:817:ARG:HE	1.51	0.76
1:B:578:VAL:HG12	1:B:581:LEU:HD22	1.66	0.75
1:B:628:PRO:HG2	1:B:742:ILE:HG13	1.68	0.75
1:C:182:CYS:HB2	1:C:257:LEU:HA	1.68	0.75
1:B:614:ILE:HD11	1:B:651:LEU:HD22	1.68	0.75
1:C:836:LYS:HD3	1:C:886:LYS:HE2	1.70	0.74
1:A:534:LEU:HA	1:A:537:GLU:HG2	1.70	0.74
1:C:493:ALA:HA	1:C:496:LYS:HD2	1.69	0.74
1:B:188:MSE:O	1:B:192:GLY:N	2.21	0.74
1:B:430:ILE:HA	1:B:433:LEU:HD23	1.70	0.73
1:A:629:SER:HA	1:A:743:VAL:HG13	1.70	0.73
1:C:507:ALA:HB1	1:C:516:ALA:HA	1.69	0.73
1:B:211:LEU:HG	1:B:219:PRO:HD3	1.70	0.73
1:B:197:VAL:HA	2:B:1001:ADP:C2	2.23	0.73
1:B:603:GLN:HB3	1:B:606:ALA:HB3	1.71	0.73
1:A:497:LEU:HA	1:A:500:LEU:HD23	1.70	0.72
1:B:397:ARG:HH21	1:B:580:ARG:HH21	1.33	0.72
1:B:442:ILE:HB	1:C:517:ALA:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:HG2	2:A:1001:ADP:HN61	1.54	0.72
1:B:407:SER:OG	1:C:734:ARG:NH2	2.22	0.72
1:A:483:GLU:HA	1:A:486:ARG:HD2	1.72	0.72
1:C:628:PRO:HB2	1:C:742:ILE:HG13	1.69	0.72
1:A:798:LEU:HD21	1:A:844:PRO:HG3	1.70	0.72
1:A:630:PHE:O	1:A:745:MSE:N	2.23	0.72
1:C:579:THR:HG23	1:C:580:ARG:HG3	1.71	0.72
1:A:419:VAL:HG22	1:A:423:ARG:HG3	1.72	0.72
1:B:618:ARG:HG3	1:B:651:LEU:HD11	1.72	0.71
1:A:578:VAL:HG12	1:A:581:LEU:HD22	1.72	0.71
1:B:200:ARG:CG	2:B:1001:ADP:HN61	2.04	0.71
1:B:198:ILE:HG23	1:B:199:GLY:H	1.54	0.71
1:B:200:ARG:HD2	1:B:203:GLU:OE1	1.90	0.71
1:A:402:ARG:NH1	1:B:733:GLY:O	2.24	0.71
1:B:233:VAL:HG11	1:B:293:PHE:CD2	2.26	0.71
1:B:497:LEU:HA	1:B:500:LEU:HD23	1.73	0.71
1:A:640:LYS:NZ	1:A:747:SER:O	2.19	0.70
1:B:810:ARG:HD3	1:B:855:LEU:HD22	1.72	0.70
1:C:543:ALA:HA	1:C:546:ASN:HB3	1.72	0.70
1:A:423:ARG:HB3	1:A:558:THR:HA	1.74	0.70
1:A:211:LEU:HG	1:A:219:PRO:HD3	1.73	0.69
1:B:534:LEU:HA	1:B:537:GLU:HG2	1.74	0.69
1:B:224:GLU:OE1	1:B:696:ARG:NH2	2.25	0.69
1:C:483:GLU:HA	1:C:486:ARG:HD2	1.74	0.69
1:A:506:ASP:HA	1:A:509:ARG:HB2	1.74	0.69
1:C:321:LEU:HD13	1:C:350:ARG:HG2	1.74	0.69
1:C:634:GLY:HA3	1:C:795:PHE:HB2	1.75	0.69
1:C:394:LEU:HD23	1:C:570:VAL:HG21	1.74	0.69
1:B:433:LEU:HD21	1:B:473:LEU:HD21	1.75	0.68
1:C:771:GLU:O	1:C:775:ASN:ND2	2.26	0.68
1:A:628:PRO:HD2	1:A:742:ILE:HA	1.75	0.68
1:C:200:ARG:NH2	1:C:357:LYS:O	2.24	0.68
1:C:317:LEU:HD13	1:C:321:LEU:HD12	1.75	0.68
1:A:364:THR:O	1:A:368:LEU:N	2.24	0.68
1:B:220:VAL:HG13	1:B:353:GLN:HA	1.75	0.68
1:C:211:LEU:HD22	1:C:327:HIS:HB3	1.74	0.68
1:C:409:VAL:HA	1:C:412:ILE:HG22	1.75	0.68
1:A:213:ARG:HB2	1:A:217:ASN:HB3	1.74	0.68
1:C:420:ARG:HA	1:C:423:ARG:HD2	1.75	0.68
1:A:545:LEU:HA	1:A:548:ASN:HB2	1.75	0.68
1:B:568:GLU:OE1	1:B:568:GLU:N	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:ASP:HA	1:C:509:ARG:HB2	1.74	0.68
1:B:715:VAL:HA	1:B:718:VAL:HG22	1.75	0.68
1:A:233:VAL:HA	1:A:236:LEU:HB3	1.76	0.68
1:A:185:MSE:HG2	1:A:256:SER:HB3	1.75	0.67
1:A:634:GLY:HA3	1:A:795:PHE:HB2	1.75	0.67
1:A:397:ARG:HH21	1:A:580:ARG:HH21	1.39	0.67
1:B:571:ALA:HB2	1:B:578:VAL:HG13	1.77	0.67
1:B:810:ARG:NH2	1:B:852:GLN:HB2	2.09	0.67
1:B:405:PRO:O	1:B:409:VAL:HG13	1.94	0.67
1:A:578:VAL:HA	1:A:581:LEU:HD13	1.76	0.67
1:A:410:ASP:OD1	1:B:213:ARG:NH2	2.28	0.67
1:B:663:MSE:HB2	1:B:707:ALA:HB3	1.75	0.67
1:A:632:PHE:N	1:A:745:MSE:O	2.27	0.67
1:B:182:CYS:HB2	1:B:257:LEU:HA	1.74	0.67
1:C:630:PHE:HB2	1:C:744:VAL:HG12	1.77	0.67
1:C:690:GLN:O	1:C:690:GLN:NE2	2.27	0.67
1:C:773:VAL:O	1:C:777:LEU:N	2.22	0.67
1:C:639:GLY:N	2:C:1002:ADP:O1A	2.28	0.66
1:C:599:ILE:HG23	1:C:600:VAL:HG23	1.77	0.66
1:A:417:ALA:HA	1:A:420:ARG:HD2	1.76	0.66
1:A:486:ARG:HD3	1:A:537:GLU:HB3	1.76	0.66
1:C:434:GLU:OE2	1:C:477:ARG:NH1	2.28	0.66
1:A:402:ARG:O	1:A:407:SER:HB2	1.96	0.66
1:C:603:GLN:HB3	1:C:606:ALA:HB3	1.77	0.66
1:B:506:ASP:HA	1:B:509:ARG:HB2	1.78	0.66
1:C:829:VAL:HG12	1:C:880:VAL:HB	1.77	0.66
1:A:630:PHE:HB2	1:A:744:VAL:HG12	1.76	0.65
1:A:319:PRO:O	1:A:323:ARG:N	2.22	0.65
1:B:368:LEU:HD13	1:B:409:VAL:HG12	1.78	0.65
1:C:396:ALA:O	1:C:400:THR:OG1	2.13	0.65
1:C:695:LEU:O	1:C:739:LYS:NZ	2.21	0.65
1:C:578:VAL:HA	1:C:581:LEU:HD13	1.79	0.65
1:A:515:ARG:HD2	1:A:519:LEU:HD11	1.78	0.65
1:B:406:ASP:HA	1:B:409:VAL:HG22	1.79	0.65
1:B:777:LEU:HD22	1:B:781:PHE:HE2	1.62	0.65
1:C:882:LEU:HD12	1:C:886:LYS:HB3	1.77	0.65
1:A:228:GLY:O	1:A:232:ILE:N	2.29	0.65
1:A:420:ARG:HA	1:A:423:ARG:HD2	1.78	0.65
1:B:360:SER:N	1:B:363:GLU:HB2	2.12	0.65
1:B:213:ARG:HB2	1:B:217:ASN:HB3	1.80	0.64
1:B:458:ARG:O	1:B:462:ALA:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ARG:HH11	1:B:734:ARG:HB2	1.63	0.64
1:C:732:GLN:O	1:C:734:ARG:NE	2.27	0.64
1:C:871:GLN:HE22	1:C:890:LEU:HD11	1.61	0.64
1:A:175:ASN:O	1:A:179:SER:N	2.24	0.64
1:B:770:ARG:O	1:B:774:MSE:HG2	1.98	0.64
1:B:200:ARG:NH2	1:B:359:PRO:HD3	2.12	0.64
1:A:769:THR:HG23	1:A:772:LEU:HD13	1.79	0.64
1:B:237:ALA:HA	1:B:240:ILE:HB	1.79	0.64
1:B:364:THR:O	1:B:368:LEU:N	2.23	0.64
1:A:423:ARG:HD3	1:A:424:GLU:N	2.12	0.64
1:B:446:ALA:HB2	1:C:518:ASP:HA	1.79	0.64
1:C:695:LEU:HB3	1:C:739:LYS:HD3	1.78	0.64
1:C:200:ARG:O	1:C:204:ILE:HG12	1.98	0.63
1:A:186:THR:HA	1:A:189:ALA:HB3	1.79	0.63
1:B:260:GLY:HA3	1:C:343:LYS:HB3	1.80	0.63
1:B:254:LEU:HA	1:B:291:ILE:O	1.99	0.63
1:A:889:VAL:HG13	1:A:891:PRO:HD3	1.81	0.63
1:C:417:ALA:HA	1:C:420:ARG:HD2	1.80	0.63
1:B:280:LEU:HD23	1:B:320:MSE:HE3	1.78	0.63
1:B:298:HIS:HB3	1:B:332:THR:HG21	1.80	0.63
1:C:345:ALA:O	1:C:349:ARG:HB2	1.98	0.63
1:C:408:ALA:O	1:C:412:ILE:N	2.30	0.63
1:C:426:GLN:HG2	1:C:480:TYR:HE1	1.63	0.63
1:A:618:ARG:HG3	1:A:651:LEU:HD11	1.79	0.63
1:B:332:THR:OG1	1:B:336:GLU:HG3	1.98	0.63
1:C:672:LEU:HD21	1:C:711:ALA:HA	1.79	0.63
1:A:823:ARG:HB2	1:A:874:GLU:HG3	1.80	0.63
1:A:708:VAL:HB	1:A:747:SER:HA	1.81	0.63
1:B:662:ASP:HB3	1:B:665:GLU:HG2	1.81	0.63
1:C:419:VAL:HG22	1:C:423:ARG:HG3	1.81	0.63
1:A:882:LEU:HD12	1:A:886:LYS:HB3	1.81	0.62
1:B:219:PRO:HD2	1:B:328:CYS:O	1.99	0.62
1:B:419:VAL:HB	1:B:561:VAL:HG23	1.82	0.62
1:B:379:HIS:CA	1:B:420:ARG:HH12	2.06	0.62
1:A:599:ILE:HG23	1:A:600:VAL:HG23	1.82	0.62
1:A:789:ILE:HG12	1:A:790:SER:N	2.14	0.62
1:C:497:LEU:HA	1:C:500:LEU:HD23	1.82	0.62
1:C:784:GLU:HG3	1:C:788:ARG:HE	1.64	0.62
1:A:240:ILE:HG12	1:A:245:VAL:HB	1.81	0.62
1:A:825:VAL:HG22	1:A:874:GLU:HA	1.82	0.62
1:B:629:SER:HA	1:B:743:VAL:HG13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:889:VAL:HG13	1:B:891:PRO:HD3	1.82	0.62
1:A:816:LYS:HA	1:A:819:THR:HG22	1.82	0.62
1:B:188:MSE:HB3	1:B:193:LYS:HB3	1.82	0.62
1:B:194:ILE:HG21	1:B:234:GLU:HB3	1.82	0.62
1:B:229:LYS:HE2	1:B:331:ALA:HB1	1.81	0.62
1:C:188:MSE:O	1:C:192:GLY:N	2.30	0.62
1:B:359:PRO:HD2	1:B:405:PRO:HG2	1.82	0.61
1:A:320:MSE:SE	1:A:324:GLY:HA3	2.50	0.61
1:B:434:GLU:HA	1:B:437:LEU:HG	1.80	0.61
1:B:375:TYR:CD2	1:C:214:ARG:HD3	2.35	0.61
1:C:426:GLN:OE1	1:C:477:ARG:NH1	2.32	0.61
1:C:569:ILE:HG12	1:C:572:ARG:HH21	1.64	0.61
1:C:889:VAL:HG13	1:C:891:PRO:HD3	1.82	0.61
1:A:798:LEU:HB2	1:A:842:TYR:HB2	1.81	0.61
1:C:257:LEU:HB2	1:C:292:LEU:HD11	1.82	0.61
1:C:826:ILE:HG23	1:C:877:VAL:HA	1.82	0.61
1:B:211:LEU:HA	1:B:217:ASN:O	1.99	0.61
1:B:226:GLY:C	1:B:406:ASP:HB2	2.21	0.61
1:B:569:ILE:O	1:B:573:TRP:HB2	2.01	0.61
1:A:666:TYR:HE2	1:A:674:ARG:HD2	1.65	0.61
1:C:227:VAL:HA	1:C:405:PRO:HG2	1.83	0.61
1:C:611:SER:OG	1:C:615:ARG:NH2	2.21	0.61
1:B:608:GLN:O	1:B:612:ASN:N	2.32	0.61
1:C:628:PRO:HD2	1:C:742:ILE:HA	1.82	0.61
1:B:423:ARG:HB3	1:B:558:THR:HA	1.82	0.60
1:C:294:VAL:HG21	1:C:300:LEU:HD11	1.83	0.60
1:B:599:ILE:HG23	1:B:600:VAL:HG23	1.82	0.60
1:C:273:GLU:HA	1:C:276:MSE:HB2	1.82	0.60
1:B:426:GLN:HG2	1:B:480:TYR:HE1	1.66	0.60
1:B:197:VAL:HA	2:B:1001:ADP:N1	2.16	0.60
1:B:652:PHE:HZ	1:B:702:ILE:HG23	1.66	0.60
1:B:866:LEU:HD12	1:B:871:GLN:HB2	1.84	0.60
1:C:358:GLU:HB2	1:C:403:ARG:NE	2.15	0.60
1:C:437:LEU:HD22	1:C:469:VAL:HG21	1.84	0.60
1:C:836:LYS:HD2	1:C:882:LEU:HD11	1.84	0.60
1:A:259:VAL:O	1:A:263:VAL:HG23	2.02	0.60
1:A:851:LEU:O	1:A:855:LEU:HB2	2.01	0.60
1:C:486:ARG:HD3	1:C:537:GLU:HB3	1.82	0.60
1:B:784:GLU:HG3	1:B:788:ARG:HE	1.67	0.59
1:C:184:ASP:HA	1:C:255:LEU:HA	1.83	0.59
1:C:457:ALA:O	1:C:461:GLN:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:ARG:HB3	1:C:510:MSE:SE	2.52	0.59
1:A:732:GLN:O	1:A:734:ARG:NE	2.29	0.59
1:B:567:ASN:HB3	1:B:578:VAL:HG11	1.83	0.59
1:B:871:GLN:HE22	1:B:890:LEU:HD11	1.67	0.59
1:A:798:LEU:HD23	1:A:842:TYR:HD1	1.68	0.59
1:B:720:LEU:HA	1:B:723:MSE:SE	2.53	0.59
1:C:601:VAL:HG11	1:C:805:LYS:HD3	1.85	0.59
1:C:798:LEU:HD21	1:C:844:PRO:HG3	1.84	0.59
1:A:774:MSE:HE2	1:A:786:LEU:HD23	1.85	0.59
1:B:402:ARG:HG2	1:C:733:GLY:O	2.02	0.59
1:A:677:GLY:O	1:A:692:THR:HA	2.03	0.59
1:B:420:ARG:HE	1:C:212:SER:HB2	1.67	0.59
1:B:490:ILE:HD11	1:B:533:ARG:HB2	1.84	0.59
1:C:497:LEU:HD13	1:C:526:GLU:HG2	1.83	0.59
1:C:715:VAL:HA	1:C:718:VAL:HG22	1.84	0.59
1:B:404:LEU:HB3	1:B:405:PRO:HD3	1.85	0.59
1:B:415:ALA:O	1:B:561:VAL:HG21	2.02	0.59
1:B:578:VAL:HA	1:B:581:LEU:HD13	1.83	0.59
1:B:319:PRO:O	1:B:323:ARG:N	2.32	0.59
1:A:863:LEU:HD23	1:B:621:LEU:HD11	1.85	0.59
1:C:403:ARG:HH12	1:C:696:ARG:HH12	1.51	0.59
1:A:211:LEU:HA	1:A:217:ASN:O	2.03	0.58
1:A:300:LEU:HB3	1:A:314:ALA:HB2	1.85	0.58
1:B:207:VAL:HA	1:B:210:ILE:HD12	1.84	0.58
1:A:231:THR:HA	1:A:234:GLU:HB2	1.83	0.58
1:B:777:LEU:HB3	1:B:781:PHE:HD2	1.67	0.58
1:A:853:ARG:NH2	1:B:792:VAL:HG22	2.19	0.58
1:B:379:HIS:NE2	1:B:413:ASP:OD1	2.34	0.58
1:A:441:LYS:O	1:A:444:ILE:HG12	2.02	0.58
1:A:579:THR:HG23	1:A:580:ARG:HG3	1.84	0.58
1:A:715:VAL:HA	1:A:718:VAL:HG22	1.85	0.58
1:B:414:GLU:OE1	1:C:732:GLN:NE2	2.37	0.58
1:A:178:LEU:N	1:A:282:GLU:OE1	2.35	0.58
1:B:640:LYS:NZ	1:B:747:SER:O	2.28	0.58
1:C:568:GLU:HA	1:C:571:ALA:HB3	1.86	0.58
1:B:219:PRO:HG2	1:B:329:ILE:HG23	1.86	0.58
1:C:666:TYR:HE2	1:C:674:ARG:HD2	1.69	0.58
1:B:399:LEU:HD11	1:C:732:GLN:HB2	1.85	0.58
1:C:400:THR:HA	1:C:403:ARG:HA	1.84	0.58
1:A:781:PHE:HB2	1:A:786:LEU:HD11	1.86	0.58
1:B:216:LYS:HB3	1:B:352:GLN:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:ILE:HB	1:B:459:LEU:HD22	1.86	0.58
1:B:437:LEU:HD22	1:B:469:VAL:HG21	1.85	0.58
1:C:608:GLN:O	1:C:612:ASN:N	2.34	0.58
1:B:816:LYS:HA	1:B:819:THR:HG22	1.84	0.57
1:A:771:GLU:O	1:A:775:ASN:ND2	2.37	0.57
1:B:183:ILE:O	1:B:256:SER:N	2.32	0.57
1:B:224:GLU:OE1	1:B:357:LYS:HG3	2.04	0.57
1:B:359:PRO:O	1:B:364:THR:HG23	2.04	0.57
1:B:831:GLU:O	1:B:835:ASP:N	2.36	0.57
1:C:280:LEU:HD23	1:C:320:MSE:HE3	1.85	0.57
1:C:823:ARG:HB2	1:C:874:GLU:HG3	1.85	0.57
1:B:196:PRO:HA	1:B:238:GLN:HE22	1.70	0.57
1:B:717:THR:O	1:B:721:GLN:N	2.29	0.57
1:C:843:SER:HB3	1:C:847:GLY:O	2.04	0.57
1:A:810:ARG:NH2	1:A:852:GLN:HB2	2.20	0.57
1:A:817:ARG:O	1:A:821:ASN:ND2	2.26	0.57
1:B:206:ARG:O	1:B:209:ARG:N	2.37	0.57
1:B:667:GLN:HA	1:B:710:LYS:HD2	1.85	0.57
1:B:854:LEU:HD13	1:B:857:LYS:HB3	1.85	0.57
1:A:379:HIS:HE1	1:B:214:ARG:HB2	1.69	0.57
1:A:490:ILE:HD11	1:A:533:ARG:HB2	1.85	0.57
1:B:347:PHE:O	1:B:351:PHE:HB2	2.05	0.57
1:B:420:ARG:NE	1:C:212:SER:HB2	2.20	0.57
1:B:426:GLN:HG2	1:B:480:TYR:CE1	2.39	0.57
1:A:773:VAL:O	1:A:777:LEU:N	2.21	0.57
1:B:379:HIS:HE2	1:C:214:ARG:HB2	1.70	0.57
1:B:777:LEU:HB2	1:B:786:LEU:HD21	1.87	0.57
1:C:185:MSE:HE1	1:C:194:ILE:HG13	1.85	0.57
1:B:378:HIS:CG	1:C:214:ARG:HG3	2.40	0.57
1:B:216:LYS:HD3	1:B:352:GLN:HB3	1.87	0.57
1:C:568:GLU:O	1:C:572:ARG:N	2.27	0.57
1:A:719:LEU:HD21	1:A:745:MSE:HE2	1.87	0.57
1:B:228:GLY:O	1:B:231:THR:OG1	2.17	0.57
1:B:228:GLY:HA2	2:B:1001:ADP:O2A	2.05	0.57
1:B:413:ASP:HB3	1:C:213:ARG:HE	1.68	0.57
1:A:459:LEU:HD13	1:A:463:LYS:HG3	1.87	0.56
1:A:568:GLU:O	1:A:572:ARG:N	2.25	0.56
1:B:292:LEU:HD23	1:B:294:VAL:HG12	1.87	0.56
1:A:229:LYS:HG3	1:A:331:ALA:HB1	1.85	0.56
1:A:854:LEU:HD13	1:A:857:LYS:HB3	1.85	0.56
1:B:239:ARG:HB3	1:B:244:ASP:OD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ALA:HB2	1:B:411:LEU:HD22	1.88	0.56
1:C:774:MSE:HE1	1:C:792:VAL:HG11	1.86	0.56
1:C:777:LEU:HB3	1:C:781:PHE:HD2	1.70	0.56
1:A:185:MSE:HE2	1:A:234:GLU:HG2	1.87	0.56
1:A:484:ARG:HH12	1:A:488:LYS:HE2	1.70	0.56
1:B:227:VAL:O	2:B:1001:ADP:C8	2.56	0.56
1:C:837:LEU:O	1:C:841:GLY:N	2.39	0.56
1:A:317:LEU:HD13	1:A:321:LEU:HD12	1.86	0.56
1:A:866:LEU:HD12	1:A:871:GLN:HB2	1.86	0.56
1:C:638:THR:HG23	1:C:848:ALA:HB2	1.87	0.56
1:B:798:LEU:HD21	1:B:844:PRO:HG3	1.87	0.56
1:B:383:ILE:HG12	1:B:561:VAL:O	2.05	0.56
1:B:627:PRO:O	1:B:629:SER:N	2.38	0.56
1:A:853:ARG:HH21	1:B:792:VAL:H	1.52	0.56
1:C:358:GLU:HB2	1:C:403:ARG:HE	1.71	0.56
1:C:423:ARG:HB3	1:C:558:THR:HA	1.88	0.56
1:A:421:VAL:HG11	1:B:209:ARG:HE	1.71	0.56
1:B:421:VAL:HG22	1:C:209:ARG:HH21	1.71	0.56
1:C:220:VAL:HG11	1:C:337:TYR:HE1	1.71	0.56
1:C:402:ARG:O	1:C:407:SER:HB2	2.05	0.56
1:B:231:THR:HA	1:B:234:GLU:HB2	1.87	0.56
1:A:229:LYS:HA	1:A:232:ILE:HD12	1.88	0.56
1:A:321:LEU:HD22	1:A:350:ARG:HG2	1.88	0.56
1:C:219:PRO:HG2	1:C:329:ILE:HG12	1.87	0.56
1:C:228:GLY:HA3	2:C:1001:ADP:H8	1.71	0.56
1:A:479:LYS:HA	1:A:482:ARG:HB2	1.88	0.55
1:C:318:LYS:HB2	1:C:319:PRO:HD3	1.88	0.55
1:B:200:ARG:O	1:B:204:ILE:HG12	2.07	0.55
1:B:293:PHE:HE2	1:B:331:ALA:HB2	1.65	0.55
1:C:199:GLY:HA3	1:C:367:ILE:HD11	1.88	0.55
1:C:679:PRO:HG2	1:C:682:TYR:CE1	2.42	0.55
1:A:228:GLY:HA3	2:A:1001:ADP:H8	1.70	0.55
1:B:321:LEU:HD22	1:B:350:ARG:HG2	1.88	0.55
1:C:406:ASP:HA	1:C:409:VAL:HG22	1.88	0.55
1:B:798:LEU:HD23	1:B:842:TYR:HD1	1.71	0.55
1:C:629:SER:HA	1:C:743:VAL:HG13	1.89	0.55
1:C:359:PRO:HB2	1:C:363:GLU:HB3	1.88	0.55
1:C:458:ARG:O	1:C:462:ALA:HB3	2.07	0.55
1:C:851:LEU:O	1:C:855:LEU:HB2	2.06	0.55
1:A:177:ASN:N	1:A:282:GLU:OE2	2.38	0.55
1:B:820:ASP:OD1	1:B:821:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:ALA:HA	1:A:496:LYS:HD2	1.89	0.55
1:B:419:VAL:HG22	1:B:423:ARG:HG3	1.88	0.55
1:C:817:ARG:O	1:C:821:ASN:ND2	2.37	0.55
1:B:718:VAL:O	1:B:722:LEU:HB2	2.07	0.55
1:C:814:ILE:O	1:C:818:LEU:HB2	2.06	0.55
1:B:371:LEU:HD12	2:B:1001:ADP:H2'	1.89	0.55
1:B:769:THR:HG23	1:B:772:LEU:HD13	1.90	0.54
1:A:294:VAL:HG13	1:A:330:GLY:HA2	1.88	0.54
1:B:695:LEU:HD22	1:B:739:LYS:HG2	1.90	0.54
1:B:493:ALA:HA	1:B:496:LYS:HD2	1.87	0.54
1:C:593:GLU:OE2	1:C:611:SER:HB2	2.07	0.54
1:C:233:VAL:HA	1:C:236:LEU:HB3	1.89	0.54
1:C:854:LEU:HD13	1:C:857:LYS:HB3	1.89	0.54
1:A:321:LEU:HD11	1:A:351:PHE:HE1	1.72	0.54
1:B:851:LEU:O	1:B:855:LEU:HB2	2.08	0.54
1:B:853:ARG:NH2	1:C:792:VAL:HG22	2.23	0.54
1:A:199:GLY:HA3	1:A:367:ILE:HD11	1.89	0.54
1:A:814:ILE:HA	1:A:817:ARG:HE	1.73	0.54
1:B:652:PHE:CZ	1:B:702:ILE:HG23	2.42	0.54
1:B:691:LEU:HD11	1:B:705:PHE:HZ	1.72	0.54
1:B:843:SER:HB3	1:B:847:GLY:O	2.08	0.54
1:C:231:THR:HA	1:C:234:GLU:HB2	1.90	0.54
1:C:531:ILE:O	1:C:535:GLU:HG2	2.07	0.54
1:A:562:GLY:H	1:A:565:GLN:HB2	1.72	0.54
1:A:641:THR:HG23	1:A:704:LEU:HD13	1.88	0.54
1:B:594:GLN:O	1:B:598:LYS:HB2	2.07	0.54
1:C:360:SER:N	1:C:363:GLU:HB2	2.23	0.54
1:C:846:TYR:O	1:C:849:ARG:NH1	2.39	0.54
1:A:631:LEU:HD22	1:A:745:MSE:SE	2.57	0.54
1:C:441:LYS:NZ	1:C:441:LYS:O	2.31	0.54
1:C:774:MSE:HE2	1:C:786:LEU:HD23	1.90	0.54
1:B:617:GLN:HG2	1:B:628:PRO:HD3	1.90	0.53
1:A:478:GLU:O	1:A:482:ARG:N	2.41	0.53
1:B:418:ALA:HA	1:C:209:ARG:CZ	2.39	0.53
1:C:403:ARG:HH22	1:C:696:ARG:HH22	1.55	0.53
1:B:543:ALA:HA	1:B:546:ASN:HB3	1.90	0.53
1:C:270:GLY:C	1:C:272:PHE:H	2.11	0.53
1:A:605:GLU:HA	1:A:608:GLN:HB2	1.90	0.53
1:A:434:GLU:HA	1:A:437:LEU:HG	1.91	0.53
1:B:300:LEU:HB3	1:B:314:ALA:HB2	1.91	0.53
1:B:378:HIS:CB	1:C:214:ARG:HG3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:577:PRO:O	1:C:579:THR:HG22	2.09	0.53
1:C:691:LEU:HD11	1:C:705:PHE:HZ	1.74	0.53
1:C:769:THR:HG23	1:C:772:LEU:HD13	1.90	0.53
1:A:640:LYS:HZ2	1:A:748:ASN:HA	1.74	0.53
1:A:660:ARG:NH1	1:B:784:GLU:OE1	2.42	0.53
1:C:478:GLU:O	1:C:482:ARG:N	2.42	0.53
1:A:663:MSE:SE	1:A:705:PHE:HB3	2.58	0.53
1:B:291:ILE:HA	1:B:327:HIS:O	2.08	0.53
1:A:705:PHE:O	1:A:746:THR:OG1	2.20	0.53
1:B:864:ALA:HB2	1:C:621:LEU:HG	1.90	0.53
1:C:652:PHE:HB3	1:C:700:PHE:HB3	1.91	0.53
1:A:476:LEU:O	1:A:480:TYR:HB3	2.08	0.53
1:B:184:ASP:HA	1:B:255:LEU:HA	1.89	0.53
1:B:254:LEU:HD21	1:B:293:PHE:HB3	1.90	0.53
1:B:339:LYS:HD3	1:B:340:TYR:CZ	2.44	0.53
1:A:421:VAL:HG11	1:B:209:ARG:NE	2.24	0.53
1:C:537:GLU:HA	1:C:540:ALA:HB3	1.89	0.53
1:C:652:PHE:HZ	1:C:702:ILE:HG12	1.74	0.53
1:C:866:LEU:HB3	1:C:871:GLN:HB3	1.91	0.53
1:A:381:VAL:HG13	1:A:419:VAL:HG11	1.91	0.52
1:B:264:ALA:O	1:B:275:ARG:NH2	2.36	0.52
1:B:437:LEU:O	1:B:441:LYS:N	2.41	0.52
1:B:716:LEU:HD22	1:B:719:LEU:HD23	1.92	0.52
1:C:397:ARG:HH22	1:C:652:PHE:C	2.13	0.52
1:A:383:ILE:HG21	1:A:387:ALA:HB3	1.90	0.52
1:B:420:ARG:HG2	1:B:421:VAL:N	2.24	0.52
1:B:420:ARG:HA	1:B:423:ARG:HH11	1.74	0.52
1:C:476:LEU:O	1:C:480:TYR:HB3	2.09	0.52
1:A:406:ASP:HA	1:A:409:VAL:HG22	1.91	0.52
1:B:228:GLY:HA2	2:B:1001:ADP:PA	2.49	0.52
1:B:262:LEU:HD13	1:B:276:MSE:SE	2.60	0.52
1:B:198:ILE:HG21	1:B:367:ILE:HA	1.91	0.52
1:B:490:ILE:HA	1:B:493:ALA:HB3	1.89	0.52
1:B:617:GLN:O	1:B:623:ASN:ND2	2.41	0.52
1:A:828:LYS:HG2	1:A:879:HIS:NE2	2.24	0.52
1:B:337:TYR:CE1	1:B:353:GLN:HB3	2.45	0.52
1:C:594:GLN:O	1:C:598:LYS:HB2	2.10	0.52
1:A:230:THR:N	2:A:1001:ADP:O3B	2.43	0.52
1:B:280:LEU:HD21	1:B:316:LEU:HB3	1.92	0.52
1:A:301:MSE:SE	1:A:301:MSE:H	2.43	0.52
1:A:400:THR:HA	1:A:403:ARG:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:ALA:HB1	1:A:577:PRO:HA	1.90	0.52
2:B:1001:ADP:N3	2:B:1001:ADP:H2'	2.23	0.52
1:B:228:GLY:HA2	2:B:1001:ADP:O5'	2.09	0.52
1:B:394:LEU:HD23	1:B:570:VAL:HG21	1.92	0.52
1:B:568:GLU:HA	1:B:571:ALA:HB3	1.90	0.52
1:A:379:HIS:HA	1:A:420:ARG:HH22	1.74	0.52
1:A:577:PRO:O	1:A:579:THR:HG22	2.10	0.52
1:A:695:LEU:O	1:A:739:LYS:NZ	2.34	0.52
1:A:652:PHE:HZ	1:A:702:ILE:HG12	1.73	0.52
1:B:270:GLY:C	1:B:272:PHE:H	2.11	0.52
1:B:657:SER:HB3	1:B:701:SER:HA	1.91	0.52
1:A:525:PRO:O	1:A:529:ALA:N	2.38	0.52
1:A:828:LYS:HG2	1:A:879:HIS:CE1	2.45	0.52
1:B:570:VAL:HB	1:B:581:LEU:HD21	1.91	0.52
1:B:611:SER:O	1:B:615:ARG:NE	2.43	0.52
1:B:262:LEU:O	1:B:275:ARG:NH2	2.42	0.52
1:C:234:GLU:O	1:C:238:GLN:HB2	2.10	0.52
1:C:423:ARG:HD3	1:C:424:GLU:N	2.24	0.52
1:A:360:SER:H	1:A:363:GLU:HB2	1.75	0.52
1:C:493:ALA:O	1:C:496:LYS:HB2	2.10	0.52
1:A:196:PRO:HB3	1:A:238:GLN:HE22	1.76	0.51
1:A:627:PRO:O	1:A:629:SER:N	2.44	0.51
1:B:197:VAL:HG11	1:B:231:THR:O	2.10	0.51
1:B:441:LYS:O	1:B:444:ILE:HG12	2.09	0.51
1:B:481:GLU:HA	1:B:484:ARG:HB2	1.92	0.51
1:A:639:GLY:HA2	1:A:642:LEU:HB3	1.92	0.51
1:A:666:TYR:CE2	1:A:674:ARG:HD2	2.46	0.51
1:A:568:GLU:OE1	1:A:568:GLU:N	2.28	0.51
1:A:414:GLU:HB3	1:A:569:ILE:HD13	1.93	0.51
1:A:426:GLN:HG2	1:A:480:TYR:HE1	1.76	0.51
1:A:573:TRP:HA	1:A:573:TRP:CE3	2.46	0.51
1:A:442:ILE:HG22	1:B:517:ALA:HB2	1.91	0.51
1:B:562:GLY:N	1:B:565:GLN:HB2	2.12	0.51
1:C:220:VAL:HG13	1:C:353:GLN:HA	1.91	0.51
1:A:414:GLU:O	1:A:418:ALA:N	2.44	0.51
1:B:220:VAL:HG11	1:B:337:TYR:HE1	1.76	0.51
1:B:421:VAL:CG2	1:C:209:ARG:HH21	2.23	0.51
1:C:789:ILE:HG12	1:C:791:SER:H	1.76	0.51
1:A:468:ASN:OD1	1:A:469:VAL:N	2.41	0.51
1:B:375:TYR:CE2	1:C:214:ARG:HD3	2.45	0.51
1:B:605:GLU:O	1:B:609:SER:N	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:708:VAL:HG13	1:C:746:THR:O	2.10	0.51
1:A:360:SER:N	1:A:363:GLU:HB2	2.25	0.51
1:C:229:LYS:HG3	1:C:331:ALA:HB1	1.92	0.51
1:C:436:ARG:HG3	1:C:437:LEU:HD23	1.91	0.51
1:B:253:LYS:O	1:B:290:ILE:HG12	2.11	0.51
1:C:526:GLU:CD	1:C:526:GLU:H	2.14	0.51
1:A:296:ALA:HA	1:A:332:THR:HB	1.93	0.51
1:A:481:GLU:HA	1:A:484:ARG:HB2	1.93	0.51
1:B:537:GLU:HG3	1:B:538:LYS:N	2.25	0.51
1:C:211:LEU:HG	1:C:219:PRO:CD	2.40	0.51
1:A:361:ILE:HG12	1:A:396:ALA:HB2	1.91	0.51
1:B:228:GLY:HA3	2:B:1001:ADP:C8	2.46	0.51
1:B:573:TRP:HA	1:B:573:TRP:CE3	2.46	0.51
1:B:789:ILE:O	1:B:789:ILE:HG12	2.11	0.51
1:B:871:GLN:HE22	1:B:890:LEU:HD21	1.76	0.51
1:A:567:ASN:HB3	1:A:578:VAL:HG11	1.92	0.50
1:B:353:GLN:N	1:B:353:GLN:OE1	2.44	0.50
1:A:453:GLU:O	1:A:456:LYS:NZ	2.36	0.50
1:A:559:ASP:OD1	1:A:559:ASP:N	2.44	0.50
1:A:719:LEU:O	1:A:723:MSE:HG2	2.12	0.50
1:B:397:ARG:HH12	1:B:652:PHE:HA	1.74	0.50
1:B:706:ASP:HA	1:B:746:THR:OG1	2.11	0.50
1:C:339:LYS:HD3	1:C:340:TYR:CZ	2.47	0.50
1:C:573:TRP:HA	1:C:573:TRP:CE3	2.46	0.50
1:A:394:LEU:HD23	1:A:570:VAL:HG21	1.92	0.50
1:B:782:LEU:HD12	1:B:784:GLU:HB3	1.92	0.50
1:B:817:ARG:O	1:B:821:ASN:ND2	2.27	0.50
1:C:568:GLU:OE1	1:C:568:GLU:N	2.44	0.50
1:B:628:PRO:HG2	1:B:742:ILE:CG1	2.41	0.50
1:C:228:GLY:O	1:C:232:ILE:HG12	2.11	0.50
1:C:641:THR:HG23	1:C:704:LEU:HD13	1.93	0.50
1:C:777:LEU:HD22	1:C:781:PHE:HE2	1.75	0.50
1:A:318:LYS:HB2	1:A:319:PRO:HD3	1.92	0.50
1:B:301:MSE:HG3	1:B:314:ALA:HB3	1.92	0.50
1:B:486:ARG:HD3	1:B:537:GLU:HB3	1.94	0.50
1:C:211:LEU:HG	1:C:219:PRO:HD3	1.93	0.50
1:A:291:ILE:HA	1:A:327:HIS:O	2.12	0.50
1:C:299:LEU:O	1:C:312:ASP:HB2	2.12	0.50
1:C:567:ASN:HB3	1:C:578:VAL:HG11	1.92	0.50
1:C:677:GLY:O	1:C:692:THR:HA	2.11	0.50
1:C:825:VAL:HG22	1:C:874:GLU:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ARG:NH2	1:C:696:ARG:HH22	2.10	0.50
1:C:464:GLN:HA	1:C:467:GLN:HB2	1.92	0.50
1:A:271:GLU:O	1:A:275:ARG:HD3	2.11	0.50
1:A:397:ARG:HH12	1:A:652:PHE:HA	1.75	0.50
1:B:618:ARG:NH2	1:B:651:LEU:HG	2.27	0.50
1:C:224:GLU:HG3	1:C:225:PRO:N	2.27	0.50
1:A:651:LEU:HD23	1:A:742:ILE:HG21	1.93	0.50
1:C:627:PRO:O	1:C:629:SER:N	2.45	0.50
1:A:561:VAL:HA	1:A:565:GLN:HG3	1.94	0.49
1:B:299:LEU:HG	1:B:303:ALA:HA	1.95	0.49
1:B:464:GLN:HA	1:B:467:GLN:HB2	1.95	0.49
1:B:708:VAL:HG13	1:B:746:THR:O	2.12	0.49
1:A:197:VAL:HG22	1:A:235:GLY:HA3	1.93	0.49
1:C:262:LEU:HA	1:C:275:ARG:HH21	1.76	0.49
1:C:294:VAL:HG13	1:C:330:GLY:HA2	1.95	0.49
1:C:773:VAL:HG12	1:C:777:LEU:HG	1.95	0.49
1:A:268:TYR:HB2	1:A:271:GLU:OE1	2.12	0.49
1:B:379:HIS:NE2	1:C:214:ARG:HB2	2.28	0.49
1:B:515:ARG:HD2	1:B:519:LEU:HD11	1.93	0.49
1:C:379:HIS:CA	1:C:420:ARG:HH12	2.26	0.49
1:C:652:PHE:CZ	1:C:702:ILE:HG23	2.47	0.49
1:A:301:MSE:SE	1:A:301:MSE:N	2.95	0.49
1:A:420:ARG:HA	1:A:423:ARG:HH11	1.77	0.49
1:A:773:VAL:HA	1:A:776:THR:OG1	2.12	0.49
1:A:810:ARG:HD3	1:A:855:LEU:HD22	1.95	0.49
1:A:814:ILE:HG13	1:A:817:ARG:NE	2.25	0.49
1:B:691:LEU:O	1:B:695:LEU:N	2.46	0.49
1:C:219:PRO:HD2	1:C:328:CYS:O	2.12	0.49
1:C:419:VAL:HG13	1:C:423:ARG:NH1	2.26	0.49
1:C:580:ARG:HA	1:C:583:THR:HB	1.95	0.49
1:B:237:ALA:O	1:B:241:VAL:HG22	2.13	0.49
1:B:338:ARG:HA	1:B:342:GLU:OE1	2.13	0.49
1:B:632:PHE:N	1:B:745:MSE:O	2.44	0.49
1:C:386:ALA:HA	1:C:389:VAL:HG22	1.95	0.49
1:C:579:THR:O	1:C:583:THR:OG1	2.15	0.49
1:C:581:LEU:HD12	1:C:581:LEU:H	1.78	0.49
1:C:592:MSE:HG2	1:C:593:GLU:OE1	2.12	0.49
1:C:651:LEU:HD23	1:C:742:ILE:HG21	1.95	0.49
1:A:691:LEU:HD11	1:A:705:PHE:HZ	1.78	0.49
1:B:425:SER:O	1:B:426:GLN:HG3	2.13	0.49
1:C:205:ARG:CZ	1:C:205:ARG:HB3	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:662:ASP:HB3	1:C:665:GLU:HG2	1.95	0.49
1:A:409:VAL:HA	1:A:412:ILE:HG22	1.93	0.49
1:A:608:GLN:OE1	1:A:612:ASN:ND2	2.42	0.49
1:B:245:VAL:HG21	1:B:250:ALA:HA	1.93	0.49
1:B:321:LEU:HD13	1:B:350:ARG:HG2	1.95	0.49
1:B:397:ARG:HG3	1:B:398:TYR:CE2	2.48	0.49
1:B:524:ILE:H	1:B:524:ILE:HD13	1.77	0.49
1:C:500:LEU:HD21	1:C:526:GLU:HG3	1.94	0.49
1:C:611:SER:HG	1:C:615:ARG:HH21	1.54	0.49
1:A:367:ILE:HG23	2:A:1001:ADP:C2	2.48	0.49
1:A:262:LEU:HB3	1:A:272:PHE:CE1	2.48	0.49
1:A:826:ILE:HG23	1:A:877:VAL:HA	1.94	0.49
1:B:213:ARG:HH12	1:B:352:GLN:NE2	2.10	0.49
1:B:337:TYR:HA	1:B:341:ILE:HG13	1.93	0.49
1:B:399:LEU:HD22	1:C:734:ARG:HH21	1.78	0.49
1:A:437:LEU:HD22	1:A:469:VAL:HG21	1.94	0.48
1:B:198:ILE:N	2:B:1001:ADP:N1	2.55	0.48
1:B:365:ILE:O	1:B:369:ARG:N	2.44	0.48
1:C:271:GLU:O	1:C:275:ARG:HD3	2.13	0.48
1:C:663:MSE:HB2	1:C:707:ALA:HB3	1.95	0.48
1:B:337:TYR:CD2	1:B:341:ILE:HB	2.48	0.48
1:B:651:LEU:HD23	1:B:742:ILE:HG21	1.94	0.48
1:C:775:ASN:O	1:C:778:ARG:HB2	2.13	0.48
1:C:668:GLU:O	1:C:672:LEU:HB2	2.12	0.48
1:C:403:ARG:HH12	1:C:696:ARG:NH1	2.11	0.48
1:C:810:ARG:HD3	1:C:855:LEU:HD22	1.95	0.48
1:A:227:VAL:HA	1:A:405:PRO:HG2	1.95	0.48
1:B:860:LEU:O	1:B:863:LEU:HB3	2.13	0.48
1:C:341:ILE:O	1:C:347:PHE:HB3	2.13	0.48
1:C:559:ASP:N	1:C:559:ASP:OD1	2.47	0.48
1:B:854:LEU:HA	1:B:857:LYS:HB2	1.95	0.48
1:C:365:ILE:HD13	1:C:389:VAL:HG12	1.95	0.48
1:C:390:ALA:O	1:C:394:LEU:HB2	2.14	0.48
1:C:695:LEU:HD22	1:C:739:LYS:HG2	1.95	0.48
1:A:197:VAL:HG11	1:A:231:THR:O	2.14	0.48
1:B:265:GLY:HA3	1:B:275:ARG:HH12	1.78	0.48
1:C:197:VAL:HG23	2:C:1001:ADP:N6	2.28	0.48
1:C:667:GLN:HA	1:C:710:LYS:HD2	1.95	0.48
1:C:866:LEU:HD12	1:C:871:GLN:HB2	1.95	0.48
1:A:270:GLY:C	1:A:272:PHE:H	2.17	0.48
1:A:823:ARG:NH1	1:A:867:ILE:HG21	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:THR:N	2:C:1001:ADP:O3B	2.47	0.48
1:C:420:ARG:HG2	1:C:421:VAL:H	1.78	0.48
1:C:630:PHE:O	1:C:745:MSE:N	2.38	0.48
1:A:378:HIS:CG	1:B:214:ARG:HG3	2.48	0.48
1:B:559:ASP:OD1	1:B:559:ASP:N	2.47	0.48
1:A:853:ARG:NH2	1:B:792:VAL:H	2.12	0.48
1:B:828:LYS:HG2	1:B:879:HIS:NE2	2.29	0.48
1:C:781:PHE:HB2	1:C:786:LEU:HD11	1.95	0.48
1:A:200:ARG:O	1:A:204:ILE:HG12	2.14	0.48
1:B:231:THR:O	1:B:235:GLY:N	2.33	0.48
1:C:358:GLU:OE2	1:C:403:ARG:HG3	2.14	0.48
1:C:379:HIS:O	1:C:420:ARG:NH1	2.43	0.48
1:C:569:ILE:HG12	1:C:572:ARG:NH2	2.29	0.48
1:A:407:SER:O	1:A:411:LEU:HB2	2.13	0.47
1:C:237:ALA:HA	1:C:240:ILE:HB	1.96	0.47
1:A:229:LYS:HG2	2:A:1001:ADP:O3B	2.14	0.47
1:A:371:LEU:HA	1:A:371:LEU:HD23	1.71	0.47
1:A:226:GLY:O	1:A:405:PRO:HB2	2.13	0.47
1:B:581:LEU:HD12	1:B:581:LEU:H	1.78	0.47
1:C:219:PRO:O	1:C:329:ILE:HA	2.14	0.47
1:A:446:ALA:HB2	1:B:518:ASP:HA	1.96	0.47
1:B:493:ALA:HB1	1:B:530:ILE:HG22	1.96	0.47
1:A:708:VAL:HG12	1:A:748:ASN:OD1	2.15	0.47
1:C:423:ARG:NH2	1:C:559:ASP:OD2	2.47	0.47
1:A:283:ILE:HG23	1:A:290:ILE:HD12	1.96	0.47
1:A:444:ILE:HD12	1:A:463:LYS:HE3	1.97	0.47
1:A:467:GLN:O	1:A:470:GLU:HB3	2.14	0.47
1:B:220:VAL:HG21	1:B:337:TYR:CD1	2.49	0.47
1:B:263:VAL:HG11	1:C:343:LYS:HE3	1.95	0.47
1:A:345:ALA:O	1:A:349:ARG:HB2	2.15	0.47
1:A:490:ILE:HA	1:A:493:ALA:HB3	1.96	0.47
1:B:298:HIS:O	1:B:302:GLY:N	2.44	0.47
1:B:823:ARG:HB2	1:B:874:GLU:CG	2.45	0.47
1:A:178:LEU:HD13	1:A:282:GLU:OE1	2.15	0.47
1:A:353:GLN:N	1:A:353:GLN:OE1	2.47	0.47
1:A:710:LYS:HA	1:A:710:LYS:HD3	1.51	0.47
1:C:198:ILE:HG23	1:C:199:GLY:H	1.79	0.47
1:C:652:PHE:HZ	1:C:702:ILE:HG23	1.79	0.47
1:A:777:LEU:HB3	1:A:781:PHE:HD2	1.79	0.47
1:B:402:ARG:O	1:B:403:ARG:NE	2.48	0.47
1:A:198:ILE:HG23	1:A:199:GLY:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:GLU:HG3	1:A:586:LYS:HG2	1.96	0.47
1:B:210:ILE:O	1:B:217:ASN:HA	2.15	0.47
1:C:359:PRO:HD2	1:C:405:PRO:HG3	1.96	0.47
1:C:468:ASN:OD1	1:C:469:VAL:N	2.46	0.47
1:A:385:ASP:O	1:A:388:ILE:HG22	2.14	0.47
1:B:468:ASN:OD1	1:B:469:VAL:N	2.48	0.47
1:B:391:ALA:HB2	1:B:566:ILE:HG13	1.96	0.47
1:B:781:PHE:HB2	1:B:786:LEU:HD11	1.96	0.47
1:B:866:LEU:HB3	1:B:871:GLN:HB3	1.97	0.47
1:C:802:GLU:O	1:C:806:ILE:HG12	2.15	0.47
1:A:200:ARG:HG2	2:A:1001:ADP:N6	2.26	0.47
1:A:427:PRO:HB2	1:A:429:ILE:HG12	1.96	0.47
1:A:638:THR:HA	2:A:1002:ADP:C8	2.50	0.47
1:B:409:VAL:HG11	2:B:1001:ADP:O2'	2.15	0.47
1:B:564:ASP:O	1:B:567:ASN:N	2.48	0.47
1:B:694:ALA:HA	1:B:697:ARG:HB3	1.97	0.47
1:A:775:ASN:O	1:A:778:ARG:HB2	2.15	0.46
1:B:332:THR:CG2	1:B:336:GLU:HB2	2.44	0.46
1:B:664:SER:HA	1:B:710:LYS:HG3	1.96	0.46
1:C:387:ALA:O	1:C:391:ALA:N	2.48	0.46
1:C:383:ILE:HG21	1:C:387:ALA:HB3	1.96	0.46
1:C:419:VAL:HG23	1:C:557:ILE:HG22	1.97	0.46
1:C:666:TYR:HD2	1:C:671:SER:HG	1.63	0.46
1:A:375:TYR:CD2	1:B:214:ARG:HD3	2.50	0.46
1:A:581:LEU:HD12	1:A:581:LEU:H	1.80	0.46
1:B:608:GLN:OE1	1:B:612:ASN:ND2	2.48	0.46
1:C:438:ARG:O	1:C:442:ILE:HB	2.15	0.46
1:A:337:TYR:HA	1:A:341:ILE:HG13	1.97	0.46
1:B:420:ARG:HG2	1:B:421:VAL:H	1.80	0.46
1:B:457:ALA:O	1:B:461:GLN:HB3	2.15	0.46
1:B:515:ARG:HH11	1:B:519:LEU:HD11	1.81	0.46
1:A:773:VAL:HA	1:A:776:THR:HG1	1.79	0.46
1:B:708:VAL:HB	1:B:781:PHE:HZ	1.79	0.46
1:C:241:VAL:HG23	1:C:242:ASN:OD1	2.15	0.46
1:A:287:LYS:HA	1:A:287:LYS:HD3	1.60	0.46
1:A:410:ASP:OD2	1:B:732:GLN:NE2	2.48	0.46
1:A:871:GLN:HE22	1:A:890:LEU:HD21	1.81	0.46
1:B:777:LEU:HD22	1:B:781:PHE:CE2	2.45	0.46
1:B:837:LEU:O	1:B:841:GLY:N	2.49	0.46
1:B:828:LYS:HG2	1:B:879:HIS:CE1	2.50	0.46
1:C:420:ARG:HG2	1:C:421:VAL:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:714:GLU:O	1:C:718:VAL:HG13	2.16	0.46
1:C:798:LEU:HD23	1:C:842:TYR:HD1	1.80	0.46
1:A:537:GLU:HA	1:A:540:ALA:HB3	1.96	0.46
1:A:839:ALA:HA	1:A:842:TYR:CE2	2.51	0.46
1:A:421:VAL:HG21	1:B:209:ARG:HH21	1.81	0.46
1:B:257:LEU:HB2	1:B:292:LEU:HD21	1.97	0.46
1:B:293:PHE:CZ	1:B:331:ALA:HB2	2.49	0.46
1:B:782:LEU:HG	1:B:785:PHE:H	1.81	0.46
1:B:784:GLU:O	1:B:788:ARG:HG2	2.16	0.46
1:C:366:SER:HA	1:C:369:ARG:HD2	1.97	0.46
1:C:396:ALA:HA	1:C:404:LEU:HD21	1.98	0.46
1:B:360:SER:O	1:B:364:THR:N	2.35	0.46
1:B:519:LEU:O	1:B:523:ALA:HB2	2.15	0.46
1:B:605:GLU:HA	1:B:608:GLN:HB2	1.97	0.46
1:B:863:LEU:HD23	1:C:621:LEU:HD11	1.97	0.46
1:C:777:LEU:HD22	1:C:781:PHE:CE2	2.50	0.46
1:C:848:ALA:O	1:C:851:LEU:HB3	2.16	0.46
1:B:403:ARG:HD3	1:B:403:ARG:HA	1.73	0.46
1:C:299:LEU:HG	1:C:303:ALA:HA	1.97	0.46
1:C:475:PRO:O	1:C:479:LYS:N	2.28	0.46
1:C:705:PHE:O	1:C:746:THR:OG1	2.26	0.46
1:C:476:LEU:HG	1:C:480:TYR:HB3	1.97	0.46
1:A:804:ARG:HG2	1:A:834:LYS:HE2	1.98	0.45
1:B:216:LYS:HE3	1:B:348:GLU:HG2	1.98	0.45
1:C:490:ILE:HD12	1:C:530:ILE:HG23	1.96	0.45
1:C:567:ASN:HB3	1:C:578:VAL:CG1	2.46	0.45
1:A:228:GLY:HA3	2:A:1001:ADP:C8	2.51	0.45
1:A:434:GLU:HB3	1:A:473:LEU:HD12	1.97	0.45
1:B:219:PRO:HG2	1:B:329:ILE:HG12	1.98	0.45
1:A:402:ARG:HG3	1:B:734:ARG:NE	2.32	0.45
1:C:854:LEU:HA	1:C:857:LYS:HB2	1.98	0.45
1:A:379:HIS:CE1	1:B:214:ARG:HB2	2.51	0.45
1:A:537:GLU:HG3	1:A:538:LYS:N	2.32	0.45
1:B:218:ASN:O	1:B:351:PHE:HA	2.16	0.45
1:A:632:PHE:O	1:A:746:THR:HA	2.16	0.45
1:C:292:LEU:O	1:C:329:ILE:N	2.40	0.45
1:B:425:SER:HA	1:C:246:PRO:HA	1.99	0.45
1:C:206:ARG:O	1:C:209:ARG:N	2.49	0.45
1:C:444:ILE:HD12	1:C:463:LYS:HG3	1.98	0.45
1:C:463:LYS:O	1:C:467:GLN:HB2	2.17	0.45
1:A:211:LEU:HG	1:A:219:PRO:CD	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LEU:HD21	1:A:581:LEU:HD23	1.99	0.45
1:A:644:THR:HG23	1:A:702:ILE:HD12	1.99	0.45
1:A:386:ALA:HA	1:A:389:VAL:HG22	1.99	0.45
1:A:837:LEU:O	1:A:841:GLY:N	2.49	0.45
1:B:230:THR:HG22	1:B:234:GLU:OE1	2.16	0.45
1:B:345:ALA:O	1:B:349:ARG:HB2	2.17	0.45
1:B:708:VAL:HB	1:B:781:PHE:CZ	2.52	0.45
1:C:229:LYS:HE2	1:C:331:ALA:HB1	1.99	0.45
1:A:668:GLU:O	1:A:672:LEU:HB2	2.17	0.45
1:A:695:LEU:HB3	1:A:739:LYS:HD3	1.98	0.45
1:A:723:MSE:HE1	1:A:789:ILE:HA	1.99	0.45
1:B:283:ILE:HG23	1:B:290:ILE:HG23	1.98	0.45
1:B:216:LYS:O	1:B:352:GLN:HG2	2.16	0.45
1:C:197:VAL:HG22	1:C:235:GLY:HA3	1.99	0.45
1:C:608:GLN:OE1	1:C:612:ASN:ND2	2.49	0.45
1:A:239:ARG:HB3	1:A:244:ASP:OD2	2.17	0.44
1:A:239:ARG:HB3	1:A:244:ASP:CG	2.38	0.44
1:A:402:ARG:HG2	1:B:733:GLY:HA2	2.00	0.44
1:B:690:GLN:O	1:B:690:GLN:NE2	2.49	0.44
1:C:361:ILE:HG12	1:C:396:ALA:CB	2.46	0.44
1:B:321:LEU:HB3	1:B:350:ARG:HD3	1.98	0.44
1:C:205:ARG:NH1	1:C:205:ARG:HB3	2.31	0.44
1:C:430:ILE:HG13	1:C:476:LEU:HD22	1.99	0.44
1:C:558:THR:O	1:C:560:VAL:N	2.48	0.44
1:A:266:SER:HB2	1:A:271:GLU:HG2	1.99	0.44
1:A:420:ARG:HG2	1:A:421:VAL:N	2.32	0.44
1:C:197:VAL:CG1	1:C:231:THR:HG22	2.48	0.44
1:C:784:GLU:O	1:C:788:ARG:HG2	2.18	0.44
1:C:873:ARG:N	1:C:876:GLU:OE1	2.50	0.44
1:A:185:MSE:CG	1:A:256:SER:HB3	2.45	0.44
1:A:260:GLY:HA3	1:B:344:ASP:OD1	2.17	0.44
1:A:222:ILE:HD12	1:A:334:LEU:HB3	2.00	0.44
1:A:614:ILE:HD12	1:A:614:ILE:HA	1.74	0.44
1:A:658:MSE:HG3	1:A:702:ILE:HD12	2.00	0.44
1:A:836:LYS:HD2	1:A:882:LEU:HD11	2.00	0.44
1:A:423:ARG:HD3	1:A:424:GLU:H	1.80	0.44
1:A:597:SER:HA	1:A:600:VAL:O	2.18	0.44
1:A:768:THR:HG23	1:A:769:THR:H	1.82	0.44
1:A:849:ARG:HG2	1:A:849:ARG:H	1.43	0.44
1:B:320:MSE:SE	1:B:324:GLY:HA3	2.67	0.44
1:B:361:ILE:HG12	1:B:396:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:LEU:O	1:B:480:TYR:HB3	2.18	0.44
1:A:568:GLU:HA	1:A:571:ALA:HB3	1.99	0.44
1:B:189:ALA:HB1	1:B:241:VAL:HG21	1.99	0.44
1:B:720:LEU:HD11	1:B:785:PHE:HD1	1.82	0.44
1:B:723:MSE:HE1	1:B:745:MSE:SE	2.68	0.44
1:B:798:LEU:HD23	1:B:842:TYR:CD1	2.52	0.44
1:C:666:TYR:O	1:C:672:LEU:HD13	2.18	0.44
1:C:828:LYS:HG2	1:C:879:HIS:NE2	2.33	0.44
1:A:178:LEU:O	1:A:182:CYS:N	2.46	0.44
1:B:188:MSE:HB2	1:B:194:ILE:HG12	2.00	0.44
1:B:300:LEU:O	1:B:314:ALA:N	2.51	0.44
1:B:413:ASP:CB	1:C:213:ARG:HE	2.31	0.44
1:C:178:LEU:HD11	1:C:283:ILE:HG13	1.99	0.44
1:C:337:TYR:CD2	1:C:341:ILE:HB	2.53	0.44
1:C:321:LEU:HD22	1:C:350:ARG:HG2	2.00	0.44
1:C:393:ASN:OD1	1:C:393:ASN:N	2.49	0.44
1:C:419:VAL:O	1:C:423:ARG:HG3	2.17	0.44
1:C:719:LEU:O	1:C:723:MSE:HG2	2.17	0.44
1:A:420:ARG:HE	1:B:212:SER:HB2	1.82	0.44
1:A:676:ILE:HD12	1:A:687:ALA:HB3	1.99	0.44
1:A:782:LEU:HD12	1:A:784:GLU:HB3	1.99	0.44
1:C:183:ILE:HA	1:C:183:ILE:HD12	1.89	0.44
1:C:359:PRO:HB2	1:C:363:GLU:CB	2.47	0.44
1:C:543:ALA:O	1:C:547:ALA:N	2.48	0.44
1:C:567:ASN:O	1:C:571:ALA:N	2.45	0.44
1:A:241:VAL:HG23	1:A:242:ASN:OD1	2.18	0.44
1:B:717:THR:HA	1:B:720:LEU:HB2	1.99	0.44
1:C:426:GLN:HA	1:C:480:TYR:OH	2.18	0.44
1:C:833:ALA:HA	1:C:882:LEU:HD13	1.99	0.44
1:A:371:LEU:O	1:A:375:TYR:HD1	2.01	0.43
1:A:463:LYS:O	1:A:467:GLN:HB2	2.18	0.43
1:B:406:ASP:OD2	2:B:1001:ADP:H4'	2.18	0.43
1:B:245:VAL:HG13	1:B:250:ALA:HB1	1.99	0.43
1:A:446:ALA:CB	1:B:518:ASP:HA	2.48	0.43
1:B:803:ILE:HG13	1:B:842:TYR:HB3	2.00	0.43
1:A:273:GLU:HA	1:A:276:MSE:HB2	1.99	0.43
1:A:666:TYR:O	1:A:672:LEU:HD13	2.19	0.43
1:A:262:LEU:HB3	1:A:272:PHE:CD1	2.53	0.43
1:A:299:LEU:O	1:A:312:ASP:HB2	2.18	0.43
1:A:359:PRO:CG	1:A:405:PRO:HG3	2.48	0.43
1:B:600:VAL:HG13	2:B:1002:ADP:N6	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:706:ASP:HA	1:C:746:THR:OG1	2.18	0.43
1:A:200:ARG:CG	2:A:1001:ADP:HN61	2.29	0.43
1:A:773:VAL:HG12	1:A:777:LEU:HG	2.00	0.43
1:B:266:SER:HA	1:B:271:GLU:HG2	2.01	0.43
1:A:503:LYS:NZ	1:A:519:LEU:HD13	2.33	0.43
1:B:198:ILE:HG22	2:B:1001:ADP:N1	2.33	0.43
1:C:209:ARG:HA	1:C:212:SER:OG	2.19	0.43
1:C:246:PRO:O	1:C:250:ALA:HB2	2.17	0.43
1:C:426:GLN:NE2	1:C:481:GLU:OE1	2.51	0.43
1:B:287:LYS:HD3	1:B:287:LYS:HA	1.70	0.43
1:B:419:VAL:HG21	1:B:559:ASP:HA	2.01	0.43
1:B:846:TYR:OH	1:C:771:GLU:OE2	2.34	0.43
1:C:338:ARG:HA	1:C:342:GLU:OE1	2.18	0.43
1:C:401:SER:O	1:C:402:ARG:NE	2.49	0.43
1:A:419:VAL:HA	1:A:422:ALA:HB3	2.00	0.43
1:B:402:ARG:NE	1:B:402:ARG:HA	2.33	0.43
1:B:503:LYS:NZ	1:B:519:LEU:HD13	2.34	0.43
1:C:420:ARG:HG2	1:C:421:VAL:HG12	1.99	0.43
1:C:632:PHE:O	1:C:746:THR:HA	2.19	0.43
1:A:202:GLU:H	1:A:202:GLU:HG2	1.62	0.43
1:A:197:VAL:CG1	1:A:231:THR:HG22	2.48	0.43
1:A:257:LEU:HD22	1:A:259:VAL:HG22	2.00	0.43
1:A:477:ARG:O	1:A:481:GLU:HB2	2.19	0.43
1:A:626:GLN:HA	1:A:723:MSE:O	2.17	0.43
1:B:211:LEU:HD23	1:B:217:ASN:O	2.18	0.43
1:B:298:HIS:CG	1:B:336:GLU:HB3	2.54	0.43
1:B:216:LYS:HB3	1:B:352:GLN:HG2	2.01	0.43
1:B:379:HIS:HA	1:B:420:ARG:NH1	2.15	0.43
1:B:421:VAL:HG21	1:C:205:ARG:HH22	1.84	0.43
1:B:427:PRO:HB2	1:B:429:ILE:HG12	1.99	0.43
1:C:287:LYS:HD3	1:C:287:LYS:HA	1.65	0.43
1:C:379:HIS:C	1:C:420:ARG:HH12	2.21	0.43
1:A:184:ASP:HA	1:A:255:LEU:HA	2.01	0.43
1:A:378:HIS:CB	1:B:214:ARG:HG3	2.49	0.43
1:B:341:ILE:O	1:B:347:PHE:HB3	2.19	0.43
1:B:719:LEU:HD21	1:B:745:MSE:HE3	2.00	0.43
1:B:814:ILE:HA	1:B:817:ARG:HG2	2.00	0.43
1:B:271:GLU:O	1:B:275:ARG:HD3	2.18	0.43
1:B:337:TYR:HA	1:B:341:ILE:CG1	2.48	0.43
1:B:345:ALA:HB1	1:B:349:ARG:HD3	2.01	0.43
1:B:421:VAL:CG2	1:C:205:ARG:HH22	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:ALA:HA	1:C:496:LYS:CD	2.46	0.43
1:C:685:HIS:CG	1:C:686:ASP:H	2.36	0.43
1:A:567:ASN:HB3	1:A:578:VAL:CG1	2.49	0.42
1:A:666:TYR:HB3	1:A:671:SER:O	2.19	0.42
1:B:834:LYS:O	1:B:838:GLY:N	2.46	0.42
1:C:711:ALA:HB1	1:C:716:LEU:HB2	2.01	0.42
1:B:226:GLY:O	1:B:406:ASP:HB2	2.19	0.42
1:B:456:LYS:HB2	1:B:456:LYS:HE3	1.93	0.42
1:A:846:TYR:OH	1:B:771:GLU:OE2	2.26	0.42
1:C:301:MSE:HG3	1:C:314:ALA:HB3	2.01	0.42
1:C:365:ILE:HD11	1:C:389:VAL:HA	2.00	0.42
1:C:381:VAL:HG13	1:C:419:VAL:HG11	2.00	0.42
1:B:407:SER:CB	1:C:734:ARG:HH22	2.32	0.42
1:A:188:MSE:HA	1:A:191:GLU:HB3	2.00	0.42
1:A:205:ARG:HB3	1:A:205:ARG:CZ	2.50	0.42
1:A:691:LEU:O	1:A:695:LEU:N	2.50	0.42
1:B:312:ASP:OD1	1:B:312:ASP:N	2.52	0.42
1:B:386:ALA:HB3	1:B:563:PRO:HD3	2.00	0.42
1:C:635:PRO:HG3	1:C:797:ARG:HA	2.01	0.42
1:A:337:TYR:HA	1:A:341:ILE:CG1	2.50	0.42
1:A:391:ALA:HB2	1:A:566:ILE:HG13	2.01	0.42
1:A:798:LEU:H	1:A:798:LEU:HD22	1.84	0.42
1:A:601:VAL:HG11	1:A:805:LYS:HD3	2.02	0.42
1:A:865:ILE:O	1:A:869:ARG:N	2.50	0.42
1:B:471:GLU:HB3	1:B:472:GLU:OE2	2.19	0.42
1:B:658:MSE:HB2	1:B:702:ILE:HD11	2.00	0.42
1:A:188:MSE:HB3	1:A:193:LYS:HB3	2.01	0.42
1:A:206:ARG:O	1:A:209:ARG:N	2.52	0.42
1:A:420:ARG:NH1	1:A:420:ARG:HB3	2.34	0.42
1:C:652:PHE:CZ	1:C:702:ILE:HG12	2.55	0.42
1:A:561:VAL:HG13	1:A:565:GLN:HB2	2.00	0.42
1:A:789:ILE:HG12	1:A:790:SER:H	1.81	0.42
1:B:393:ASN:OD1	1:B:393:ASN:N	2.53	0.42
1:B:577:PRO:O	1:B:579:THR:HG22	2.19	0.42
1:B:679:PRO:HG2	1:B:682:TYR:CE1	2.55	0.42
1:C:532:LYS:HE3	1:C:532:LYS:HB3	1.84	0.42
1:A:229:LYS:HG2	2:A:1001:ADP:PB	2.60	0.42
1:A:183:ILE:HD12	1:A:183:ILE:HA	1.84	0.42
1:A:186:THR:HA	1:A:189:ALA:CB	2.48	0.42
1:B:597:SER:HA	1:B:600:VAL:O	2.19	0.42
1:C:341:ILE:HA	1:C:347:PHE:HD2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:LEU:HD23	1:A:842:TYR:CD1	2.52	0.42
1:C:420:ARG:O	1:C:424:GLU:HB2	2.19	0.42
1:A:714:GLU:O	1:A:718:VAL:HG13	2.20	0.42
1:A:720:LEU:HD21	1:A:785:PHE:HD1	1.85	0.42
1:B:181:PHE:CZ	1:B:275:ARG:HG2	2.54	0.42
1:B:299:LEU:HG	1:B:312:ASP:OD2	2.20	0.42
1:B:320:MSE:O	1:B:325:GLN:N	2.53	0.42
1:B:831:GLU:OE1	1:B:834:LYS:HD2	2.20	0.42
1:A:420:ARG:HG2	1:A:421:VAL:H	1.84	0.42
1:B:230:THR:O	1:B:233:VAL:HG22	2.20	0.42
1:B:420:ARG:O	1:B:424:GLU:HB2	2.20	0.42
1:B:483:GLU:OE2	1:B:541:ALA:HA	2.19	0.42
1:B:610:VAL:HA	1:B:630:PHE:CE2	2.55	0.42
1:B:695:LEU:HB3	1:B:739:LYS:HD3	2.02	0.42
1:C:419:VAL:HG13	1:C:423:ARG:HH11	1.84	0.42
1:A:494:LYS:O	1:A:497:LEU:N	2.52	0.41
1:A:607:VAL:HG22	1:A:643:LEU:HD11	2.02	0.41
1:B:419:VAL:HG22	1:B:423:ARG:CG	2.50	0.41
1:C:388:ILE:HA	1:C:391:ALA:HB3	2.02	0.41
1:C:459:LEU:O	1:C:463:LYS:N	2.39	0.41
1:A:233:VAL:HG21	1:A:293:PHE:CD2	2.56	0.41
1:A:401:SER:O	1:A:402:ARG:NE	2.53	0.41
1:A:603:GLN:OE1	1:A:796:ASN:N	2.43	0.41
1:B:642:LEU:HG	2:B:1002:ADP:C4	2.55	0.41
1:B:390:ALA:O	1:B:394:LEU:HD13	2.20	0.41
1:B:429:ILE:O	1:B:433:LEU:HB3	2.20	0.41
1:C:228:GLY:O	1:C:232:ILE:N	2.50	0.41
1:A:379:HIS:HA	1:A:420:ARG:NH2	2.35	0.41
1:B:652:PHE:HB3	1:B:700:PHE:HB3	2.02	0.41
1:C:420:ARG:HB3	1:C:420:ARG:NH1	2.35	0.41
1:A:197:VAL:HG23	2:A:1001:ADP:N6	2.36	0.41
1:A:299:LEU:HG	1:A:303:ALA:HA	2.02	0.41
1:A:564:ASP:O	1:A:567:ASN:N	2.53	0.41
1:B:188:MSE:SE	1:B:194:ILE:HG12	2.70	0.41
1:B:227:VAL:HG12	1:B:405:PRO:HD2	2.02	0.41
1:B:361:ILE:HA	1:B:364:THR:HG1	1.85	0.41
1:B:407:SER:O	1:B:411:LEU:HB2	2.20	0.41
1:C:176:GLU:OE1	1:C:180:LYS:HD2	2.20	0.41
1:C:282:GLU:O	1:C:286:SER:HB3	2.20	0.41
1:C:386:ALA:HB3	1:C:563:PRO:HD3	2.03	0.41
1:A:452:ASP:O	1:A:454:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ALA:HB1	1:A:516:ALA:HA	2.02	0.41
1:B:226:GLY:HA3	1:B:406:ASP:CB	2.50	0.41
1:C:849:ARG:HG2	1:C:849:ARG:H	1.63	0.41
1:B:197:VAL:CG2	1:B:235:GLY:HA3	2.51	0.41
1:C:518:ASP:N	1:C:518:ASP:OD1	2.54	0.41
1:A:542:ASP:HA	1:A:545:LEU:HB2	2.02	0.41
1:B:194:ILE:CG2	1:B:234:GLU:HB3	2.49	0.41
1:B:240:ILE:HG23	1:B:251:ALA:HA	2.03	0.41
1:B:403:ARG:O	1:B:407:SER:HB2	2.21	0.41
1:B:216:LYS:HE2	1:B:734:ARG:HD3	2.01	0.41
1:B:631:LEU:HD22	1:B:745:MSE:HB2	2.02	0.41
1:B:826:ILE:HG23	1:B:877:VAL:HA	2.02	0.41
1:C:224:GLU:OE1	1:C:403:ARG:HB3	2.20	0.41
1:A:204:ILE:HD13	1:A:232:ILE:HG23	2.02	0.41
1:A:254:LEU:HG	1:A:291:ILE:HB	2.02	0.41
1:A:390:ALA:O	1:A:394:LEU:HB2	2.21	0.41
1:A:530:ILE:HD13	1:A:530:ILE:HA	1.76	0.41
1:B:254:LEU:HD21	1:B:293:PHE:H	1.86	0.41
1:B:196:PRO:HD2	1:B:374:LYS:HD3	2.03	0.41
1:C:196:PRO:HA	1:C:238:GLN:HE22	1.86	0.41
1:C:444:ILE:HD13	1:C:463:LYS:HA	2.02	0.41
1:A:378:HIS:HB2	1:B:214:ARG:HG3	2.02	0.41
1:A:644:THR:HG23	1:A:702:ILE:CD1	2.50	0.41
1:A:672:LEU:HD21	1:A:711:ALA:HA	2.02	0.41
1:B:219:PRO:O	1:B:329:ILE:HA	2.21	0.41
1:B:527:GLN:O	1:B:530:ILE:HG12	2.20	0.41
1:B:378:HIS:HB2	1:C:214:ARG:HG3	2.01	0.41
1:C:186:THR:HG21	1:C:253:LYS:HE3	2.03	0.41
1:C:426:GLN:HG2	1:C:480:TYR:CE1	2.51	0.41
1:C:666:TYR:CE2	1:C:674:ARG:HD2	2.54	0.41
1:C:823:ARG:HB2	1:C:874:GLU:CG	2.50	0.41
1:A:210:ILE:O	1:A:217:ASN:HA	2.21	0.41
1:A:769:THR:O	1:A:772:LEU:HB3	2.21	0.41
1:B:510:MSE:HE2	1:B:510:MSE:HB2	1.98	0.41
1:B:810:ARG:HD2	1:B:851:LEU:HD21	2.03	0.41
1:A:444:ILE:HD12	1:A:463:LYS:HG2	2.02	0.41
1:A:664:SER:HA	1:A:710:LYS:HG3	2.03	0.41
1:A:802:GLU:O	1:A:806:ILE:HG12	2.20	0.41
1:B:257:LEU:HD12	1:B:292:LEU:HD11	2.03	0.41
1:B:371:LEU:HD23	1:B:371:LEU:HA	1.83	0.41
1:B:463:LYS:O	1:B:467:GLN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:LYS:O	1:B:467:GLN:HB2	2.21	0.41
1:B:774:MSE:O	1:B:778:ARG:HG2	2.21	0.41
1:C:255:LEU:HD21	1:C:290:ILE:HG13	2.02	0.41
1:C:360:SER:OG	1:C:363:GLU:N	2.47	0.41
1:C:371:LEU:HD23	1:C:371:LEU:HA	1.94	0.41
1:C:368:LEU:HD21	1:C:412:ILE:HD12	2.03	0.41
1:C:661:PHE:HD2	1:C:662:ASP:H	1.68	0.41
1:C:745:MSE:HE1	1:C:789:ILE:HG21	2.03	0.41
1:A:191:GLU:OE1	1:A:193:LYS:N	2.54	0.40
1:A:400:THR:O	1:A:403:ARG:HD3	2.21	0.40
1:B:228:GLY:O	1:B:232:ILE:HD13	2.21	0.40
1:B:659:ILE:HG21	1:B:690:GLN:HE22	1.85	0.40
1:B:720:LEU:O	1:B:723:MSE:HG2	2.21	0.40
1:C:188:MSE:HB2	1:C:194:ILE:HG12	2.02	0.40
1:C:178:LEU:N	1:C:282:GLU:OE1	2.53	0.40
1:A:211:LEU:HD23	1:A:217:ASN:O	2.21	0.40
1:A:723:MSE:HG3	1:A:724:ASP:H	1.87	0.40
1:A:860:LEU:O	1:A:863:LEU:HB3	2.22	0.40
1:B:198:ILE:HG23	1:B:199:GLY:N	2.29	0.40
1:B:355:LEU:HD23	1:B:357:LYS:NZ	2.36	0.40
1:C:222:ILE:HD13	1:C:222:ILE:H	1.86	0.40
1:C:544:ALA:HB3	1:C:556:MSE:HE1	2.03	0.40
1:C:592:MSE:HE2	1:C:592:MSE:HB3	1.98	0.40
1:A:419:VAL:HG21	1:A:559:ASP:HA	2.03	0.40
1:A:845:VAL:HG13	1:A:846:TYR:CD2	2.56	0.40
1:B:366:SER:HA	1:B:369:ARG:HD2	2.03	0.40
1:B:401:SER:OG	1:B:402:ARG:N	2.54	0.40
1:B:446:ALA:HB3	1:C:521:TYR:HB3	2.04	0.40
1:B:691:LEU:HD11	1:B:705:PHE:CZ	2.56	0.40
1:B:777:LEU:CB	1:B:786:LEU:HD21	2.50	0.40
1:C:632:PHE:N	1:C:745:MSE:O	2.52	0.40
1:A:723:MSE:HG3	1:A:724:ASP:N	2.36	0.40
1:C:420:ARG:HA	1:C:423:ARG:HH11	1.86	0.40
1:C:433:LEU:O	1:C:437:LEU:HG	2.22	0.40
1:C:739:LYS:HD2	1:C:740:ASN:H	1.86	0.40
1:B:341:ILE:HA	1:B:347:PHE:CD2	2.57	0.40
1:C:436:ARG:NH2	1:C:469:VAL:HG11	2.36	0.40
1:C:456:LYS:HE3	1:C:456:LYS:HB2	1.97	0.40
1:C:669:ARG:O	1:C:673:SER:N	2.47	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	678/926 (73%)	585 (86%)	91 (13%)	2 (0%)	44	80
1	B	678/926 (73%)	594 (88%)	83 (12%)	1 (0%)	55	88
1	C	678/926 (73%)	587 (87%)	89 (13%)	2 (0%)	44	80
All	All	2034/2778 (73%)	1766 (87%)	263 (13%)	5 (0%)	51	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	403	ARG
1	A	403	ARG
1	A	525	PRO
1	C	359	PRO
1	B	426	GLN

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	571/751 (76%)	501 (88%)	70 (12%)	5	31
1	B	571/751 (76%)	494 (86%)	77 (14%)	4	28
1	C	571/751 (76%)	493 (86%)	78 (14%)	4	28
All	All	1713/2253 (76%)	1488 (87%)	225 (13%)	5	29

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	LEU
1	A	182	CYS
1	A	188	MSE
1	A	202	GLU
1	A	214	ARG
1	A	217	ASN
1	A	231	THR
1	A	244	ASP
1	A	253	LYS
1	A	255	LEU
1	A	288	GLU
1	A	290	ILE
1	A	294	VAL
1	A	301	MSE
1	A	311	MSE
1	A	315	ASN
1	A	326	LEU
1	A	333	THR
1	A	344	ASP
1	A	350	ARG
1	A	352	GLN
1	A	357	LYS
1	A	358	GLU
1	A	363	GLU
1	A	393	ASN
1	A	403	ARG
1	A	406	ASP
1	A	420	ARG
1	A	421	VAL
1	A	423	ARG
1	A	473	LEU
1	A	480	TYR
1	A	482	ARG
1	A	483	GLU
1	A	498	GLU
1	A	530	ILE
1	A	548	ASN
1	A	551	ASP
1	A	559	ASP
1	A	560	VAL
1	A	564	ASP
1	A	565	GLN
1	A	566	ILE

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Mol	Chain	Res	Type
1	A	573	TRP
1	A	579	THR
1	A	580	ARG
1	A	605	GLU
1	A	614	ILE
1	A	631	LEU
1	A	644	THR
1	A	647	LEU
1	A	658	MSE
1	A	661	PHE
1	A	690	GLN
1	A	692	THR
1	A	719	LEU
1	A	768	THR
1	A	774	MSE
1	A	789	ILE
1	A	798	LEU
1	A	801	ARG
1	A	816	LYS
1	A	818	LEU
1	A	821	ASN
1	A	832	GLU
1	A	849	ARG
1	A	856	GLU
1	A	871	GLN
1	A	886	LYS
1	A	890	LEU
1	B	178	LEU
1	B	182	CYS
1	B	183	ILE
1	B	185	MSE
1	B	188	MSE
1	B	197	VAL
1	B	220	VAL
1	B	231	THR
1	B	232	ILE
1	B	236	LEU
1	B	240	ILE
1	B	244	ASP
1	B	253	LYS
1	B	255	LEU
1	B	259	VAL

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Mol	Chain	Res	Type
1	B	290	ILE
1	B	294	VAL
1	B	301	MSE
1	B	312	ASP
1	B	315	ASN
1	B	326	LEU
1	B	333	THR
1	B	339	LYS
1	B	350	ARG
1	B	352	GLN
1	B	356	VAL
1	B	357	LYS
1	B	393	ASN
1	B	402	ARG
1	B	404	LEU
1	B	406	ASP
1	B	410	ASP
1	B	423	ARG
1	B	433	LEU
1	B	441	LYS
1	B	461	GLN
1	B	473	LEU
1	B	480	TYR
1	B	482	ARG
1	B	483	GLU
1	B	498	GLU
1	B	524	ILE
1	B	530	ILE
1	B	532	LYS
1	B	542	ASP
1	B	545	LEU
1	B	559	ASP
1	B	560	VAL
1	B	564	ASP
1	B	566	ILE
1	B	579	THR
1	B	580	ARG
1	B	605	GLU
1	B	616	LEU
1	B	631	LEU
1	B	644	THR
1	B	661	PHE

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Mol	Chain	Res	Type
1	B	690	GLN
1	B	692	THR
1	B	696	ARG
1	B	745	MSE
1	B	768	THR
1	B	775	ASN
1	B	789	ILE
1	B	798	LEU
1	B	801	ARG
1	B	816	LYS
1	B	818	LEU
1	B	821	ASN
1	B	832	GLU
1	B	852	GLN
1	B	856	GLU
1	B	869	ARG
1	B	871	GLN
1	B	873	ARG
1	B	886	LYS
1	B	890	LEU
1	C	178	LEU
1	C	182	CYS
1	C	217	ASN
1	C	222	ILE
1	C	224	GLU
1	C	231	THR
1	C	240	ILE
1	C	244	ASP
1	C	253	LYS
1	C	255	LEU
1	C	290	ILE
1	C	294	VAL
1	C	315	ASN
1	C	326	LEU
1	C	333	THR
1	C	339	LYS
1	C	350	ARG
1	C	352	GLN
1	C	353	GLN
1	C	357	LYS
1	C	367	ILE
1	C	393	ASN

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Mol	Chain	Res	Type
1	C	397	ARG
1	C	402	ARG
1	C	403	ARG
1	C	406	ASP
1	C	421	VAL
1	C	423	ARG
1	C	436	ARG
1	C	441	LYS
1	C	442	ILE
1	C	447	LEU
1	C	480	TYR
1	C	482	ARG
1	C	483	GLU
1	C	498	GLU
1	C	515	ARG
1	C	518	ASP
1	C	522	TYR
1	C	524	ILE
1	C	530	ILE
1	C	537	GLU
1	C	542	ASP
1	C	545	LEU
1	C	559	ASP
1	C	564	ASP
1	C	566	ILE
1	C	567	ASN
1	C	573	TRP
1	C	579	THR
1	C	580	ARG
1	C	592	MSE
1	C	605	GLU
1	C	616	LEU
1	C	631	LEU
1	C	644	THR
1	C	661	PHE
1	C	670	HIS
1	C	690	GLN
1	C	692	THR
1	C	706	ASP
1	C	719	LEU
1	C	745	MSE
1	C	768	THR

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Mol	Chain	Res	Type
1	C	789	ILE
1	C	796	ASN
1	C	798	LEU
1	C	801	ARG
1	C	816	LYS
1	C	818	LEU
1	C	821	ASN
1	C	849	ARG
1	C	856	GLU
1	C	869	ARG
1	C	871	GLN
1	C	873	ARG
1	C	886	LYS
1	C	890	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	HIS
1	A	565	GLN
1	A	775	ASN
1	B	690	GLN
1	B	852	GLN
1	B	871	GLN
1	C	690	GLN
1	C	871	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	A	1001	-	25,29,29	1.06	2 (8%)	24,45,45	1.58	2 (8%)
2	ADP	A	1002	-	25,29,29	1.02	1 (4%)	24,45,45	1.59	2 (8%)
2	ADP	B	1001	-	25,29,29	1.89	4 (16%)	24,45,45	2.83	11 (45%)
2	ADP	B	1002	-	25,29,29	1.03	1 (4%)	24,45,45	1.57	2 (8%)
2	ADP	C	1001	-	25,29,29	1.12	2 (8%)	24,45,45	1.61	2 (8%)
2	ADP	C	1002	-	25,29,29	1.05	1 (4%)	24,45,45	1.62	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	1001	-	-	0/12/32/32	0/3/3/3
2	ADP	A	1002	-	-	0/12/32/32	0/3/3/3
2	ADP	B	1001	-	-	0/12/32/32	0/3/3/3
2	ADP	B	1002	-	-	0/12/32/32	0/3/3/3
2	ADP	C	1001	-	-	0/12/32/32	0/3/3/3
2	ADP	C	1002	-	-	0/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	ADP	C2'-C3'	-2.00	1.48	1.53
2	A	1001	ADP	O4'-C1'	2.11	1.44	1.41
2	C	1001	ADP	O4'-C1'	2.40	1.44	1.41
2	A	1002	ADP	C5-C4	3.22	1.47	1.40
2	B	1002	ADP	C5-C4	3.24	1.47	1.40
2	C	1002	ADP	C5-C4	3.31	1.48	1.40
2	A	1001	ADP	C5-C4	3.43	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	ADP	C5-C4	3.52	1.48	1.40
2	B	1001	ADP	C5-C4	3.76	1.49	1.40
2	B	1001	ADP	O4'-C1'	4.23	1.47	1.41
2	B	1001	ADP	PB-O3A	5.85	1.69	1.60

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	ADP	N3-C2-N1	-8.44	121.51	128.86
2	C	1001	ADP	N3-C2-N1	-5.80	123.81	128.86
2	A	1001	ADP	N3-C2-N1	-5.61	123.97	128.86
2	A	1002	ADP	N3-C2-N1	-5.53	124.04	128.86
2	B	1002	ADP	N3-C2-N1	-5.40	124.16	128.86
2	C	1002	ADP	N3-C2-N1	-5.33	124.21	128.86
2	B	1001	ADP	C4-C5-N7	-5.07	104.51	109.41
2	B	1001	ADP	C4'-O4'-C1'	-4.19	105.31	109.77
2	B	1001	ADP	O2'-C2'-C3'	-3.79	99.67	111.83
2	A	1002	ADP	C4-C5-N7	-3.13	106.39	109.41
2	A	1001	ADP	C4-C5-N7	-3.12	106.40	109.41
2	C	1002	ADP	C4-C5-N7	-2.97	106.54	109.41
2	C	1001	ADP	C4-C5-N7	-2.96	106.55	109.41
2	B	1002	ADP	C4-C5-N7	-2.87	106.64	109.41
2	B	1001	ADP	O3'-C3'-C2'	-2.66	103.31	111.83
2	B	1001	ADP	O2A-PA-O5'	-2.47	96.50	108.14
2	B	1001	ADP	O3B-PB-O1B	-2.26	101.66	110.50
2	B	1001	ADP	C5-C6-N6	2.38	125.33	120.47
2	B	1001	ADP	C1'-N9-C4	2.45	130.86	126.64
2	B	1001	ADP	O3B-PB-O2B	2.69	118.46	107.61
2	B	1001	ADP	C2-N1-C6	3.22	124.40	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ADP	10	0
2	A	1002	ADP	1	0
2	B	1001	ADP	16	0
2	B	1002	ADP	2	0
2	C	1001	ADP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1002	ADP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	672/926 (72%)	-0.67	12 (1%) 69 56	133, 225, 282, 313	10 (1%)
1	B	672/926 (72%)	-0.82	4 (0%) 89 83	1, 205, 268, 309	10 (1%)
1	C	672/926 (72%)	-0.85	6 (0%) 84 74	38, 219, 272, 294	10 (1%)
All	All	2016/2778 (72%)	-0.78	22 (1%) 80 69	1, 218, 275, 313	30 (1%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	825	VAL	4.1
1	A	681	GLY	3.8
1	B	671	SER	3.4
1	A	636	SER	3.2
1	C	883	VAL	2.9
1	A	880	VAL	2.8
1	A	637	GLY	2.8
1	A	533	ARG	2.7
1	C	879	HIS	2.4
1	A	881	GLU	2.4
1	B	443	GLU	2.4
1	A	678	ALA	2.4
1	B	653	ASP	2.3
1	A	264	ALA	2.3
1	A	377	VAL	2.2
1	C	637	GLY	2.2
1	B	687	ALA	2.2
1	C	576	ILE	2.1
1	C	678	ALA	2.1
1	A	826	ILE	2.1
1	C	681	GLY	2.0
1	A	827	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ADP	B	1001	27/27	0.99	0.15	-0.29	2,6,13,16	0
2	ADP	A	1001	27/27	0.94	0.15	-0.49	173,225,244,252	0
2	ADP	C	1001	27/27	0.96	0.15	-0.50	169,220,243,244	0
2	ADP	B	1002	27/27	0.96	0.12	-0.66	214,240,243,245	0
2	ADP	A	1002	27/27	0.95	0.12	-0.69	197,248,253,257	0
2	ADP	C	1002	27/27	0.94	0.11	-0.76	198,227,236,239	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.