



Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 08:58 PM EDT

PDB ID : 6X6J / pdb_00006x6j
EMDB ID : EMD-20021
Title : Cryo-EM Structure of CagX and CagY within the Helicobacter pylori PR
Authors : Sheedlo, M.J.; Chung, J.M.; Sawhney, N.; Durie, C.L.; Cover, T.L.; Ohi, M.D.;
Lacy, D.B.
Deposited on : 2020-05-28
Resolution : 3.50 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

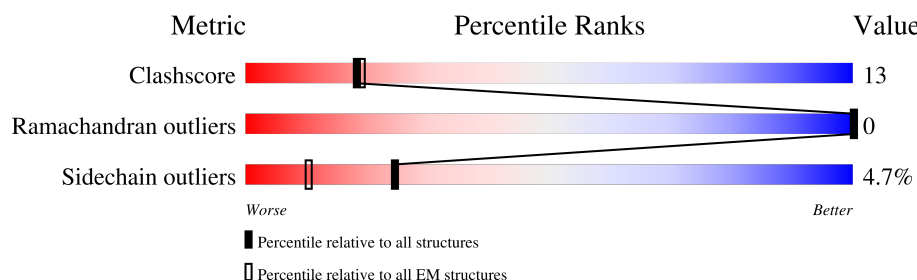
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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


















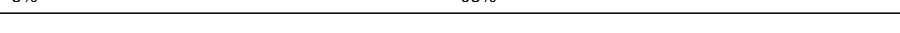
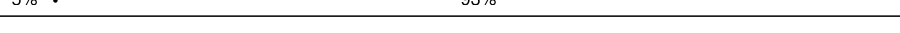
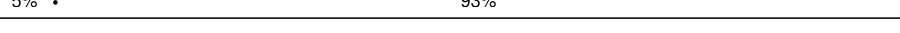
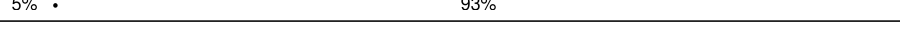
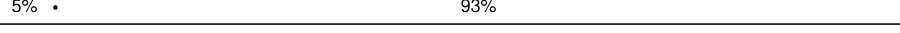
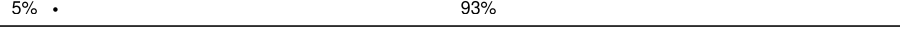
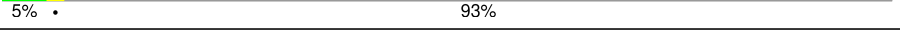


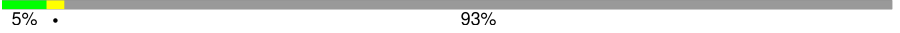
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	AX	521	
1	BX	521	
1	CX	521	
1	DX	521	
1	EX	521	
1	FX	521	
1	GX	521	
1	HX	521	
1	IX	521	

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Mol	Chain	Length	Quality of chain
1	JX	521	 19% 12% 69%
1	KX	521	 21% 10% 69%
1	LX	521	 21% 9% 69%
1	MX	521	 21% 10% 69%
1	NX	521	 20% 11% 69%
1	OX	521	 20% 11% 69%
1	PX	521	 20% 10% 69%
1	QX	521	 20% 10% 69%
2	AY	1927	 5% 93%
2	BY	1927	 5% 93%
2	CY	1927	 5% 93%
2	DY	1927	 5% 93%
2	EY	1927	 5% 93%
2	FY	1927	 5% 93%
2	GY	1927	 5% 93%
2	HY	1927	 5% 93%
2	IY	1927	 5% 93%
2	JY	1927	 5% 93%
2	KY	1927	 5% 93%
2	LY	1927	 5% 93%
2	MY	1927	 5% 93%
2	NY	1927	 5% 93%
2	OY	1927	 5% 93%
2	PY	1927	 5% 93%
2	QY	1927	 5% 93%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 40613 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cag pathogenicity island protein (Cag8).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	BX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	CX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	DX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	EX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	FX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	GX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	HX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	IX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	JX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	KX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	LX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	MX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	NX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	OX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	PX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		
1	QX	164	Total	C	N	O	S	0	0
			1339	858	227	252	2		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AX	?	-	GLU	deletion	UNP O25263
AX	516	GLU	LEU	conflict	UNP O25263
BX	?	-	GLU	deletion	UNP O25263
BX	516	GLU	LEU	conflict	UNP O25263
CX	?	-	GLU	deletion	UNP O25263
CX	516	GLU	LEU	conflict	UNP O25263
DX	?	-	GLU	deletion	UNP O25263
DX	516	GLU	LEU	conflict	UNP O25263
EX	?	-	GLU	deletion	UNP O25263
EX	516	GLU	LEU	conflict	UNP O25263
FX	?	-	GLU	deletion	UNP O25263
FX	516	GLU	LEU	conflict	UNP O25263
GX	?	-	GLU	deletion	UNP O25263
GX	516	GLU	LEU	conflict	UNP O25263
HX	?	-	GLU	deletion	UNP O25263
HX	516	GLU	LEU	conflict	UNP O25263
IX	?	-	GLU	deletion	UNP O25263
IX	516	GLU	LEU	conflict	UNP O25263
JX	?	-	GLU	deletion	UNP O25263
JX	516	GLU	LEU	conflict	UNP O25263
KX	?	-	GLU	deletion	UNP O25263
KX	516	GLU	LEU	conflict	UNP O25263
LX	?	-	GLU	deletion	UNP O25263
LX	516	GLU	LEU	conflict	UNP O25263
MX	?	-	GLU	deletion	UNP O25263
MX	516	GLU	LEU	conflict	UNP O25263
NX	?	-	GLU	deletion	UNP O25263
NX	516	GLU	LEU	conflict	UNP O25263
OX	?	-	GLU	deletion	UNP O25263
OX	516	GLU	LEU	conflict	UNP O25263
PX	?	-	GLU	deletion	UNP O25263
PX	516	GLU	LEU	conflict	UNP O25263
QX	?	-	GLU	deletion	UNP O25263
QX	516	GLU	LEU	conflict	UNP O25263

- Molecule 2 is a protein called Cag pathogenicity island protein (Cag7).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AY	135	Total	C	N	O	S	0	0
			1050	649	177	220	4		
2	BY	135	Total	C	N	O	S	0	0
			1050	649	177	220	4		

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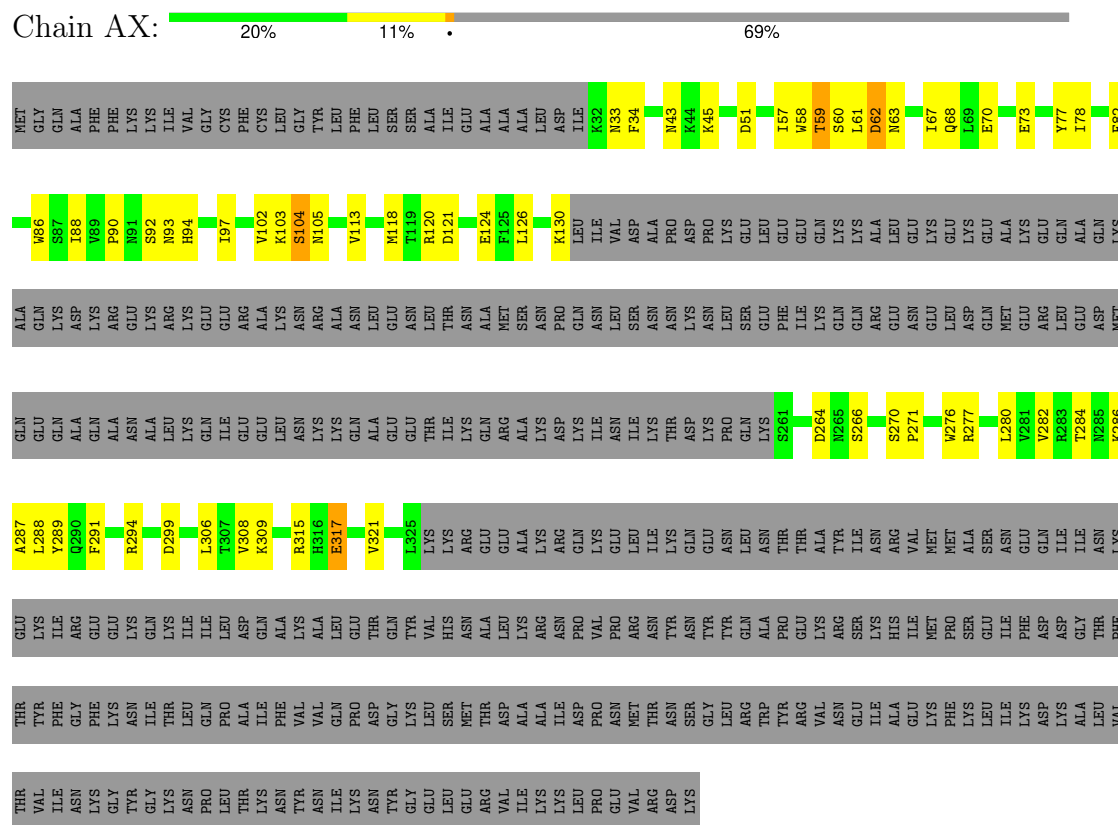
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	CY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	DY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	EY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	FY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	GY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	HY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	IY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	JY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	KY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	LY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	MY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	NY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	OY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	PY	135	Total 1050	C 649	N 177	O 220	S 4	0	0
2	QY	135	Total 1050	C 649	N 177	O 220	S 4	0	0

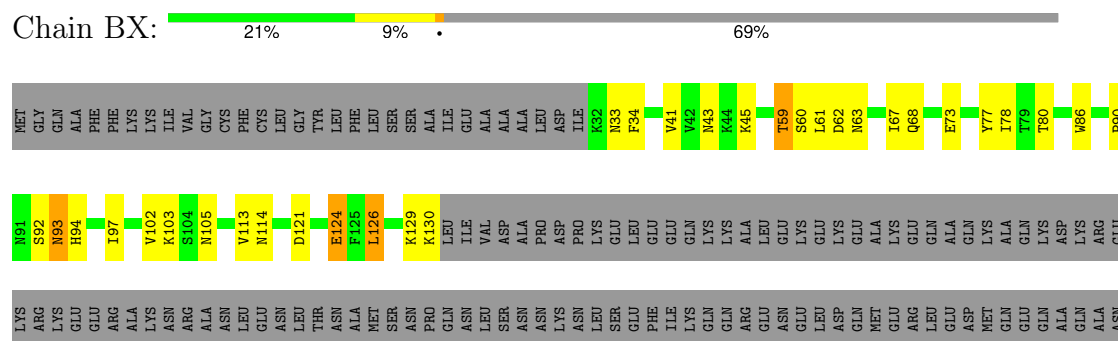
3 Residue-property plots [i](#)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

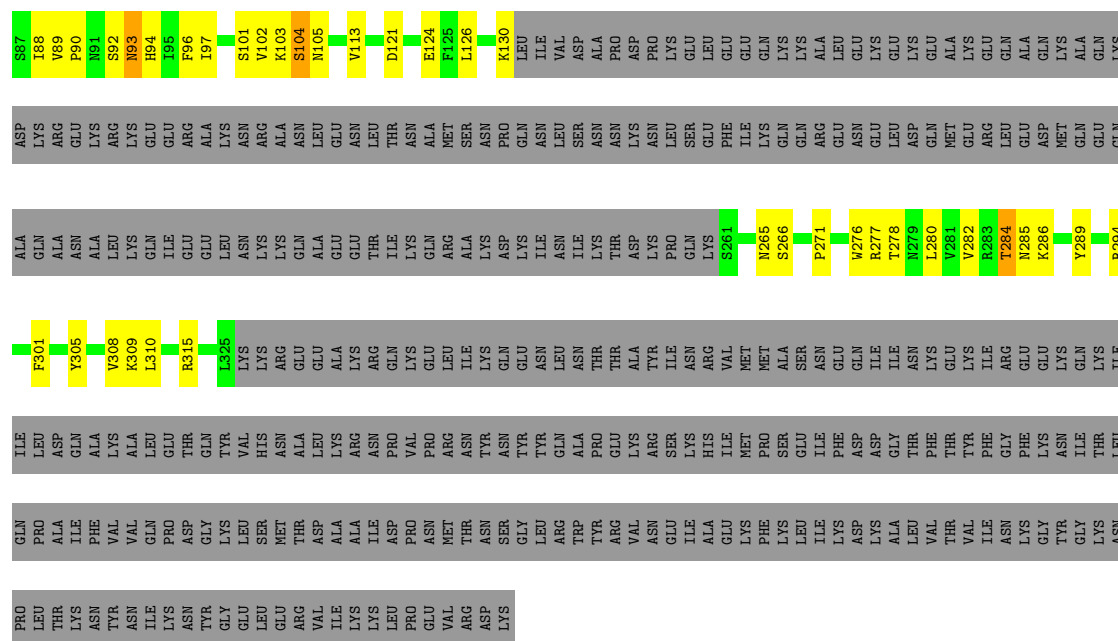
- Molecule 1: Cag pathogenicity island protein (Cag8)



- Molecule 1: Cag pathogenicity island protein (Cag8)

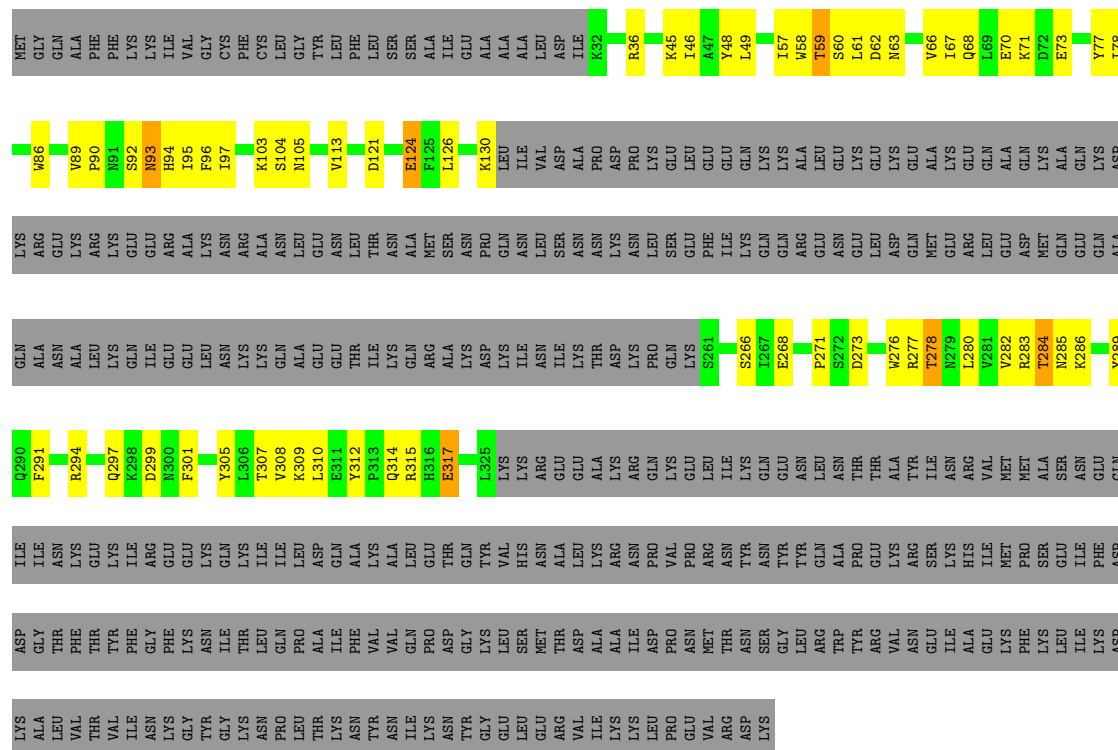






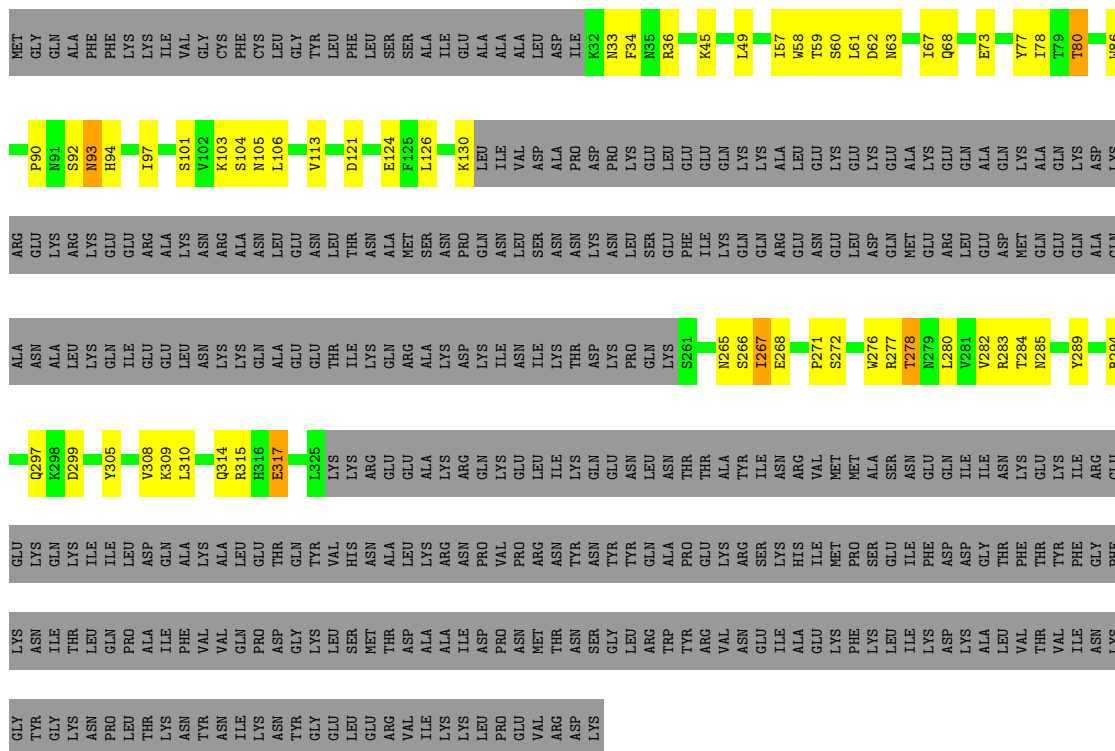
• Molecule 1: Cag pathogenicity island protein (Cag8)

Chain GX: 19% 11% • 69%

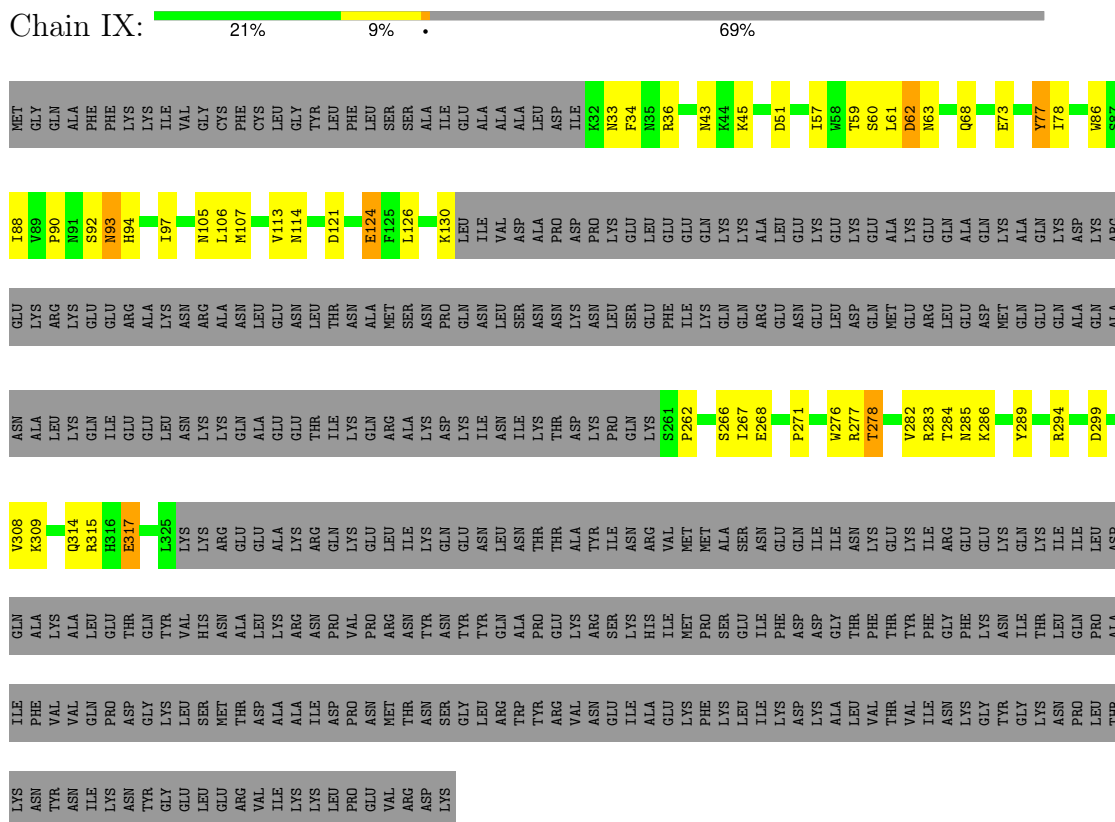


• Molecule 1: Cag pathogenicity island protein (Cag8)

Chain HX: 20% 10% • 69%



- Molecule 1: Cag pathogenicity island protein (Cag8)



- Molecule 1: Cag pathogenicity island protein (Cag8)

Category	Percentage
Very bad	19%
Bad	12%
Average	1%
Good	69%



Response	Percentage
Yes	21%
No	10%
Don't know	69%



Chain LX: 21% 9% 69%

PRO	LEU	THR	LYS	TYR	ASN	VAL	GLN	ILE	D299	Q314	K309	F301	R300	Q303	Q304	Q305	Q306	Q307	Q308	Q309	Q310	Q311	Q312	Q313	Q314	Q315	Q316	Q317	Q318	Q319	Q320	Q321	Q322	Q323	Q324	Q325	Q326	Q327	Q328	Q329	Q330	Q331	Q332	Q333	Q334	Q335	Q336	Q337	Q338	Q339	Q340	Q341	Q342	Q343	Q344	Q345	Q346	Q347	Q348	Q349	Q350	Q351	Q352	Q353	Q354	Q355	Q356	Q357	Q358	Q359	Q360	Q361	Q362	Q363	Q364	Q365	Q366	Q367	Q368	Q369	Q370	Q371	Q372	Q373	Q374	Q375	Q376	Q377	Q378	Q379	Q380	Q381	Q382	Q383	Q384	Q385	Q386	Q387	Q388	Q389	Q390	Q391	Q392	Q393	Q394	Q395	Q396	Q397	Q398	Q399	Q400	Q401	Q402	Q403	Q404	Q405	Q406	Q407	Q408	Q409	Q410	Q411	Q412	Q413	Q414	Q415	Q416	Q417	Q418	Q419	Q420	Q421	Q422	Q423	Q424	Q425	Q426	Q427	Q428	Q429	Q430	Q431	Q432	Q433	Q434	Q435	Q436	Q437	Q438	Q439	Q440	Q441	Q442	Q443	Q444	Q445	Q446	Q447	Q448	Q449	Q450	Q451	Q452	Q453	Q454	Q455	Q456	Q457	Q458	Q459	Q460	Q461	Q462	Q463	Q464	Q465	Q466	Q467	Q468	Q469	Q470	Q471	Q472	Q473	Q474	Q475	Q476	Q477	Q478	Q479	Q480	Q481	Q482	Q483	Q484	Q485	Q486	Q487	Q488	Q489	Q490	Q491	Q492	Q493	Q494	Q495	Q496	Q497	Q498	Q499	Q500	Q501	Q502	Q503	Q504	Q505	Q506	Q507	Q508	Q509	Q510	Q511	Q512	Q513	Q514	Q515	Q516	Q517	Q518	Q519	Q520	Q521	Q522	Q523	Q524	Q525	Q526	Q527	Q528	Q529	Q530	Q531	Q532	Q533	Q534	Q535	Q536	Q537	Q538	Q539	Q540	Q541	Q542	Q543	Q544	Q545	Q546	Q547	Q548	Q549	Q550	Q551	Q552	Q553	Q554	Q555	Q556	Q557	Q558	Q559	Q560	Q561	Q562	Q563	Q564	Q565	Q566	Q567	Q568	Q569	Q570	Q571	Q572	Q573	Q574	Q575	Q576	Q577	Q578	Q579	Q580	Q581	Q582	Q583	Q584	Q585	Q586	Q587	Q588	Q589	Q590	Q591	Q592	Q593	Q594	Q595	Q596	Q597	Q598	Q599	Q600	Q601	Q602	Q603	Q604	Q605	Q606	Q607	Q608	Q609	Q610	Q611	Q612	Q613	Q614	Q615	Q616	Q617	Q618	Q619	Q620	Q621	Q622	Q623	Q624	Q625	Q626	Q627	Q628	Q629	Q630	Q631	Q632	Q633	Q634	Q635	Q636	Q637	Q638	Q639	Q640	Q641	Q642	Q643	Q644	Q645	Q646	Q647	Q648	Q649	Q650	Q651	Q652	Q653	Q654	Q655	Q656	Q657	Q658	Q659	Q660	Q661	Q662	Q663	Q664	Q665	Q666	Q667	Q668	Q669	Q670	Q671	Q672	Q673	Q674	Q675	Q676	Q677	Q678	Q679	Q680	Q681	Q682	Q683	Q684	Q685	Q686	Q687	Q688	Q689	Q690	Q691	Q692	Q693	Q694	Q695	Q696	Q697	Q698	Q699	Q700	Q701	Q702	Q703	Q704	Q705	Q706	Q707	Q708	Q709	Q710	Q711	Q712	Q713	Q714	Q715	Q716	Q717	Q718	Q719	Q720	Q721	Q722	Q723	Q724	Q725	Q726	Q727	Q728	Q729	Q730	Q731
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[illegible]



PHE	THR	THR	TYR	PHE	GLY	PHE	LYS	ASN	ILE	THR	LYS	LEU	GLN	PRO	GLN	PRO	GLY	PHE	VAL	VAL	GLN	PRO	ASP	GLY	LYS	LEU	SER	MET	THR	THR	ASP	ALA	ALA	ASP	ILE	ASP	PRO	PRO	ASN	MET	THR	ASN	SER	GLY	LEU	ARG	LEU	TPP	TYR	ARG	VAL	ASN	ASN	GLY	ILE	ALA	ALA	GLY	LYS	PHE	LYS	LYS	LEU	ILE	LYS	ASP	LYS	ALA	LEU	TYR																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
VAL	THR	VAL	ILE	ASN	GLY	LYS	GLY	TYR	GLY	LYS	ASN	PRO	LEU	THR	THR	ILE	LYS	ASN	ASN	TYR	ASN	ASN	GLY	GLY	LEU	GLU	GLU	ARG	VAL	ILE	ILE	LYS	LYS	LYS	LEU	GLU	VAL	VAL	ARG	ASP	ASN	LYS	ASP	LYS	GLN	LYS	PHE	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LY

• Molecule 1: Cag pathogenicity island protein (Cag8)

Chain PX:  20% 10% 69%

LYS	PHE	GLU	R294	ALA	ARG	P90	MET
GLY	GLU	GLU		ASN	GLU		GLY
TYR	LYS	LYS	D299	ALA	LYS	H91	GLN
GLY	ILE	GLN		LEU	ARG	S92	ALA
LYS	THR	LYS	Y305	LYS	LYS	N93	PHE
ASN	LEU	ILE		GLN	GLU	H94	PHE
PRO	GLN	ILE	V308	ILE	GLU	I95	LYS
LEU	LEU	LEU	K309	GLU	ARG	F96	LYS
THR	ASP	ASP	E311	GLU	ALA		ILE
LYS	ILE	GLN	Y312	LEU	LYS	S101	VAL
ASN	PHE	ALA	P313	ASN	ASN	S104	GLY
TYR	VAL	LYS	Q314	LYS	ARG	N105	CYS
ASN	VAL	ALA	R315	LYS	ALA	L106	PHE
ILE	GLN	LEU	Q314	GLN	ASN		CYS
LYS	GLY	LEU	H316	ALA	LEU	E109	LYS
ASN	ASP	THR	E317	GLY	GLU		GLY
TYR	GLY	GLN		GLU	ASN	V113	TYR
LYS	LYS	TYR	I325	THR	LEU		LEU
GLU	LEU	VAL	LYS	ILE	THR	D121	PHE
LEU	SER	HIS	LYS	LYS	ASN		LEU
GLU	GLU	ASN	ARG	GLN	ALA	E124	SER
GLU	MET	ALA	GLU	ALA	MET	F125	SER
ARG	THR	ALA	GLU	ALA	SER	L126	ALA
VAL	ASP	LEU	GLY	LYS	ASN		ILE
ILE	ALA	LYS	ALA	ASP	PRO	K130	GLU
LYS	ALA	ARG	LYS	LYS	GLY		ALA
LYS	ILE	ASN	ARG	ILE	ASN	LEU	ALA
ASP	ASP	PRO	GLN	LYS	GLN	ILE	ASP
PRO	PRO	VAL	PRO	PRO	GLY	VAL	ALA
GLU	ASN	PRO	GLY	ILE	SER	ASP	LEU
VAL	MET	ARG	LEU	LYS	ASN	ALA	ASP
ARG	THR	ASN	ILE	THR	ASN	PRO	ASP
ASN	ASN	TYR	LYS	ASP	LYS	ASP	ILE
SER	SER	TYR	GLY	LYS	ASN	PRO	R36
GLY	GLY	TYR	GLU	PRO	LEU	LYS	G37
LEU	ARG	TYR	ASN	GLN	SER	GLU	R38
THR	THR	ALA	LEU	LYS	GLU	LEU	
ASP	ASP	PRO	ALA	ASN	PHE	GLU	K45
LYS	GLY	GLN	ASN	LYS	ILE	GLU	
ASN	ASN	ALA	ASN	GLY	LYS	GLN	T56
ARG	ARG	LYS	THR	I267	GLN	LYS	I57
ASN	ASN	ARG	TYR	ALA	GLN	LYS	W58
GLY	GLY	SER	ILE	P271	ARG	ALA	T59
ILE	ILE	LYS	ASN		ASN	LEU	S60
ALA	HIS	ARG	ARG	W276	ASN	GLU	L61
GLU	GLU	VAL	VAL	R277	GLU	LYS	D62
LYS	LYS	MET	MET	T278	LEU	GLU	N63
PHE	PHE	PRO	MET	N279	ASP	LYS	
LYS	LYS	SER	ALA	L280	GLN	GLU	Q68
LEU	LEU	GLU	SER	V281	MET	ALA	
ILE	ILE	ILE	ASN	V282	GLY	LYS	K71
LYS	LYS	PHE	GLU	R283	ARG	GLU	D72
ASP	ASP	ASP	GLN	T284	LEU	GLN	E73
LYS	LYS	ASP	ILE	N285	GLY	GLN	
ALA	ALA	GLY	ILE	K286	ASP	GLN	Y77
THR	THR	THR	ASN		MET	LYS	I78
LEU	VAL	PHE	LYS	Y289	GLN	ALA	W86
VAL	THR	THR	GLY	Q290	GLU	LYS	
VAL	VAL	TYR	LYS	F291	LYS	LYS	Y89
ASP	ASP	PHE	ILE	I292	ILE	ASP	
ILE	ASN	GLY	ASP	I293	ASP	LYS	

• Molecule 1: Cag pathogenicity island protein (Cag8)

Chain QX:  20% 10% 69%

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[illegible]

- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain AY: 5% 93%

[illegible]





	GLY	ASN
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- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain DY: 5% 93%

[illegible]



Molecule 2: Cag pathogenicity island protein (Cag7)

Chain FY: 5% .93%









[illegible]

- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain LY:  5% . 93%

[illegible]

[illegible]

- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain MY:  5% . 93%



[illegible]

ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL
VAL	LEU	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL
ALA	GLN	ALA	GLN	ALA	GLN	ALA	GLN	ALA	GLN	ALA	GLN	ALA	GLN	ALA	GLN	ALA	GLN	ALA	GLN	ALA	GLN	ALA	GLN	ALA	GLN	ALA	GLN	ALA	GLN
TYR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
PRO	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
ILE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU
ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY	ASN	GLY
ILE	THR	ILE	THR	ILE	THR	ILE	THR	ILE	THR	ILE	THR	ILE	THR	ILE	THR	ILE	THR	ILE	THR	ILE	THR	ILE	THR	ILE	THR	ILE	THR	ILE	THR
THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
SER	ALA	SER	ALA	SER	ALA	SER	ALA	SER	ALA	SER	ALA	SER	ALA	SER	ALA	SER	ALA	SER	ALA	SER	ALA	SER	ALA	SER	ALA	SER	ALA	SER	ALA
LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS	LEU	LYS
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
ASP	ASN	ASP	ASN	ASP	ASN	ASP	ASN	ASP	ASN	ASP	ASN	ASP	ASN	ASP	ASN	ASP	ASN	ASP	ASN	ASP	ASN	ASP	ASN	ASP	ASN	ASP	ASN	ASP	ASN
GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR	GLY	THR
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY	VAL	GLY
ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL	ASP	VAL
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET	MET
ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP	TRP
ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN	ASN
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY								

Tyr	Lys	Asn	Glu	Gly	Asp	Ser	Thr	Leu	Lys	Val	Ala	Pro	Arg	His	Glu	Gly	Thr	Ser	Pro	Lys	Gly	Asn
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- Molecule 2: Cag pathogenicity island protein (Cag7)

Chain OY:  5% 93%

[illegible]





[illegible]



TYR
LYS
ASN
GLU
GLY
ASP
SER
ILE
LYS
ILE
LEU
THR
MET
ASP
ASP
ILE
ASP
PHE
SER
GLY
VAL
TYR
ASP
VAL
LYS
ILE
THR
ASN
LYS
SER
VAL
VAL
ASP
GLU
ILE
ILE
LYS
GLN
SER
THR
LYS
THR
LEU
SER
ARG
GLU
HIS
GLU
GLU
ILE
THR
THR
SER
PRO
LYS
GLY
GLY
ASN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20929	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AX	0.39	0/1365	0.46	0/1845
1	BX	0.39	0/1365	0.46	0/1845
1	CX	0.39	0/1365	0.46	0/1845
1	DX	0.40	0/1365	0.46	0/1845
1	EX	0.39	0/1365	0.46	0/1845
1	FX	0.39	0/1365	0.46	0/1845
1	GX	0.39	0/1365	0.46	0/1845
1	HX	0.40	0/1365	0.46	0/1845
1	IX	0.39	0/1365	0.46	0/1845
1	JX	0.40	0/1365	0.46	0/1845
1	KX	0.39	0/1365	0.46	0/1845
1	LX	0.39	0/1365	0.46	0/1845
1	MX	0.39	0/1365	0.46	0/1845
1	NX	0.39	0/1365	0.46	0/1845
1	OX	0.39	0/1365	0.46	0/1845
1	PX	0.39	0/1365	0.46	0/1845
1	QX	0.40	0/1365	0.46	0/1845
2	AY	0.30	0/1061	0.41	0/1432
2	BY	0.30	0/1061	0.42	0/1432
2	CY	0.31	0/1061	0.43	0/1432
2	DY	0.31	0/1061	0.42	0/1432
2	EY	0.30	0/1061	0.42	0/1432
2	FY	0.30	0/1061	0.41	0/1432
2	GY	0.30	0/1061	0.42	0/1432
2	HY	0.33	0/1061	0.45	0/1432
2	IY	0.30	0/1061	0.41	0/1432
2	JY	0.31	0/1061	0.43	0/1432
2	KY	0.30	0/1061	0.42	0/1432
2	LY	0.30	0/1061	0.42	0/1432
2	MY	0.30	0/1061	0.42	0/1432
2	NY	0.30	0/1061	0.42	0/1432
2	OY	0.31	0/1061	0.42	0/1432
2	PY	0.30	0/1061	0.41	0/1432
2	QY	0.30	0/1061	0.41	0/1432

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	0/41242	0.44	0/55709

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	AX	1339	0	1355	47	0
1	BX	1339	0	1355	37	0
1	CX	1339	0	1355	54	0
1	DX	1339	0	1355	53	0
1	EX	1339	0	1355	43	0
1	FX	1339	0	1355	43	0
1	GX	1339	0	1355	48	0
1	HX	1339	0	1355	43	0
1	IX	1339	0	1355	41	0
1	JX	1339	0	1355	54	0
1	KX	1339	0	1355	40	0
1	LX	1339	0	1355	39	0
1	MX	1339	0	1355	43	0
1	NX	1339	0	1355	50	0
1	OX	1339	0	1355	42	0
1	PX	1339	0	1355	41	0
1	QX	1339	0	1355	44	0
2	AY	1050	0	1038	32	0
2	BY	1050	0	1038	36	0
2	CY	1050	0	1038	28	0
2	DY	1050	0	1038	29	0
2	EY	1050	0	1038	32	0
2	FY	1050	0	1038	28	0
2	GY	1050	0	1038	28	0
2	HY	1050	0	1038	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	IY	1050	0	1038	32	0
2	JY	1050	0	1038	32	0
2	KY	1050	0	1038	28	0
2	LY	1050	0	1038	24	0
2	MY	1050	0	1038	32	0
2	NY	1050	0	1038	29	0
2	OY	1050	0	1038	23	0
2	PY	1050	0	1038	24	0
2	QY	1050	0	1038	31	0
All	All	40613	0	40681	1048	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 13.

All (1048) 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:LX:126:LEU:O	1:LX:130:LYS:HB2	1.65	0.96
1:MX:126:LEU:O	1:MX:130:LYS:HB2	1.68	0.93
1:QX:126:LEU:O	1:QX:130:LYS:HB2	1.68	0.93
1:NX:126:LEU:O	1:NX:130:LYS:HB2	1.71	0.91
1:JX:126:LEU:O	1:JX:130:LYS:HB2	1.71	0.91
1:HX:126:LEU:O	1:HX:130:LYS:HB2	1.71	0.90
1:KX:126:LEU:O	1:KX:130:LYS:HB2	1.73	0.89
1:AX:126:LEU:O	1:AX:130:LYS:HB2	1.73	0.88
1:IX:126:LEU:O	1:IX:130:LYS:HB2	1.74	0.87
1:GX:126:LEU:O	1:GX:130:LYS:HB2	1.75	0.87
1:DX:126:LEU:O	1:DX:130:LYS:HB2	1.74	0.87
1:CX:126:LEU:O	1:CX:130:LYS:HB2	1.74	0.86
1:BX:126:LEU:O	1:BX:130:LYS:HB2	1.74	0.86
1:FX:126:LEU:O	1:FX:130:LYS:HB2	1.79	0.83
1:OX:126:LEU:O	1:OX:130:LYS:HB2	1.79	0.82
2:GY:1576:ILE:HG21	2:HY:1584:TYR:HE1	1.45	0.81
1:PX:126:LEU:O	1:PX:130:LYS:HB2	1.80	0.81
2:HY:1482:LEU:HD13	2:HY:1513:LYS:HD2	1.61	0.80
2:OY:1576:ILE:HG21	2:PY:1584:TYR:HE1	1.48	0.79
2:NY:1576:ILE:HG21	2:OY:1584:TYR:HE1	1.49	0.78
1:QX:77:TYR:HB2	1:QX:283:ARG:HH21	1.49	0.78
2:PY:1576:ILE:HG21	2:QY:1584:TYR:HE1	1.49	0.77
2:LY:1576:ILE:HG21	2:MY:1584:TYR:HE1	1.50	0.77
2:MY:1576:ILE:HG21	2:NY:1584:TYR:HE1	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:OX:284:THR:HG23	1:OX:286:LYS:H	1.50	0.76
2:KY:1576:ILE:HG21	2:LY:1584:TYR:HE1	1.49	0.76
1:DX:73:GLU:OE2	1:DX:315:ARG:NH1	2.17	0.76
1:FX:277:ARG:HD2	1:FX:294:ARG:HH11	1.49	0.76
1:EX:126:LEU:O	1:EX:130:LYS:HB2	1.85	0.76
1:AX:104:SER:HB2	2:QY:1547:PHE:HB3	1.67	0.75
2:CY:1482:LEU:HD13	2:CY:1513:LYS:HD2	1.67	0.75
1:NX:73:GLU:OE2	1:NX:315:ARG:NH1	2.18	0.75
2:BY:1576:ILE:HG21	2:CY:1584:TYR:HE1	1.50	0.75
1:KX:104:SER:HB2	2:JY:1547:PHE:HB3	1.69	0.74
1:BX:277:ARG:HD2	1:BX:294:ARG:HH11	1.52	0.74
1:QX:73:GLU:OE2	1:QX:315:ARG:NH1	2.20	0.73
2:HY:1576:ILE:HG21	2:IY:1584:TYR:HE1	1.52	0.73
1:HX:73:GLU:OE2	1:HX:315:ARG:NH1	2.16	0.73
1:NX:104:SER:HB2	2:MY:1547:PHE:HB3	1.70	0.72
2:AY:1584:TYR:HE1	2:QY:1576:ILE:HG21	1.54	0.72
1:EX:73:GLU:OE2	1:EX:315:ARG:NH1	2.21	0.72
2:DY:1576:ILE:HG21	2:EY:1584:TYR:HE1	1.52	0.72
1:LX:73:GLU:OE2	1:LX:315:ARG:NH1	2.23	0.72
1:MX:73:GLU:OE2	1:MX:315:ARG:NH1	2.23	0.72
1:BX:73:GLU:OE2	1:BX:315:ARG:NH1	2.19	0.72
1:PX:104:SER:HB2	2:OY:1547:PHE:HB3	1.72	0.71
2:OY:1482:LEU:HD13	2:OY:1513:LYS:HD2	1.71	0.71
1:FX:104:SER:HB2	2:EY:1547:PHE:HB3	1.72	0.71
1:OX:277:ARG:HD2	1:OX:294:ARG:HH11	1.53	0.70
1:MX:104:SER:HB2	2:LY:1547:PHE:HB3	1.73	0.70
1:LX:78:ILE:HG21	1:LX:90:PRO:HG3	1.72	0.70
1:IX:73:GLU:OE2	1:IX:315:ARG:NH1	2.19	0.70
1:JX:104:SER:HB2	2:IY:1547:PHE:HB3	1.71	0.70
2:FY:1533:ASP:HA	2:GY:1519:VAL:HG21	1.72	0.70
2:IY:1576:ILE:HG21	2:JY:1584:TYR:HE1	1.55	0.70
1:AX:277:ARG:HD2	1:AX:294:ARG:HH11	1.57	0.69
1:IX:78:ILE:HG21	1:IX:90:PRO:HG3	1.75	0.69
1:AX:73:GLU:OE2	1:AX:315:ARG:NH1	2.25	0.69
1:KX:277:ARG:HD2	1:KX:294:ARG:HH11	1.56	0.69
1:LX:104:SER:HB2	2:KY:1547:PHE:HB3	1.73	0.69
2:EY:1576:ILE:HG21	2:FY:1584:TYR:HE1	1.57	0.69
1:MX:78:ILE:HG21	1:MX:90:PRO:HG3	1.74	0.68
1:EX:277:ARG:HD2	1:EX:294:ARG:HH11	1.58	0.68
2:KY:1533:ASP:HA	2:LY:1519:VAL:HG21	1.76	0.68
1:HX:68:GLN:HA	1:HX:94:HIS:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JY:1482:LEU:HD13	2:JY:1513:LYS:HD2	1.76	0.67
1:JX:68:GLN:HB3	1:JX:309:LYS:HA	1.77	0.67
1:HX:277:ARG:HD2	1:HX:294:ARG:HH11	1.59	0.67
1:KX:73:GLU:OE2	1:KX:315:ARG:NH1	2.25	0.67
1:JX:73:GLU:OE2	1:JX:315:ARG:NH1	2.23	0.67
2:CY:1576:ILE:HG21	2:DY:1584:TYR:HE1	1.60	0.67
1:PX:277:ARG:HD2	1:PX:294:ARG:HH11	1.60	0.66
1:NX:277:ARG:HD2	1:NX:294:ARG:HH11	1.60	0.66
1:CX:73:GLU:OE2	1:CX:315:ARG:NH1	2.28	0.66
1:JX:277:ARG:HD2	1:JX:294:ARG:HH11	1.60	0.66
1:NX:78:ILE:HG21	1:NX:90:PRO:HG3	1.77	0.66
2:JY:1576:ILE:HG21	2:KY:1584:TYR:HE1	1.61	0.66
1:FX:61:LEU:HD22	1:FX:271:PRO:HG2	1.76	0.66
1:CX:104:SER:HB2	2:BY:1547:PHE:HB3	1.78	0.65
1:QX:67:ILE:HA	1:QX:308:VAL:HG23	1.78	0.65
1:LX:61:LEU:HD22	1:LX:271:PRO:HG2	1.78	0.65
1:FX:78:ILE:HG21	1:FX:90:PRO:HG3	1.79	0.65
1:IX:51:ASP:O	1:JX:43:ASN:ND2	2.29	0.65
1:OX:68:GLN:HB3	1:OX:309:LYS:HA	1.79	0.65
1:OX:61:LEU:HD22	1:OX:271:PRO:HG2	1.79	0.65
2:GY:1598:LYS:HA	2:GY:1601:LYS:HE3	1.80	0.64
1:GX:77:TYR:HB2	1:GX:283:ARG:HH21	1.62	0.64
1:KX:67:ILE:HA	1:KX:308:VAL:HG23	1.79	0.64
1:JX:78:ILE:HG21	1:JX:90:PRO:HG3	1.80	0.64
1:DX:104:SER:HB2	2:CY:1547:PHE:HB3	1.79	0.64
2:AY:1533:ASP:HA	2:BY:1519:VAL:HG21	1.80	0.64
1:KX:62:ASP:OD1	2:IY:1548:LYS:NZ	2.31	0.63
1:PX:78:ILE:HG21	1:PX:90:PRO:HG3	1.80	0.63
2:BY:1533:ASP:HA	2:CY:1519:VAL:HG21	1.79	0.63
1:GX:104:SER:HB2	2:FY:1547:PHE:HB3	1.80	0.63
1:BX:62:ASP:OD1	2:QY:1548:LYS:NZ	2.30	0.63
1:CX:129:LYS:O	1:DX:120:ARG:NH1	2.31	0.63
2:JY:1489:THR:O	2:JY:1491:GLN:NE2	2.31	0.63
1:DX:62:ASP:OD2	2:BY:1548:LYS:NZ	2.31	0.63
1:LX:277:ARG:HD2	1:LX:294:ARG:HH11	1.63	0.63
1:BX:105:ASN:OD1	1:BX:266:SER:OG	2.17	0.63
1:PX:105:ASN:OD1	1:PX:266:SER:OG	2.16	0.63
1:CX:51:ASP:O	1:DX:43:ASN:ND2	2.31	0.62
1:IX:77:TYR:HB2	1:IX:283:ARG:HH21	1.64	0.62
1:HX:78:ILE:HG21	1:HX:90:PRO:HG3	1.82	0.62
1:QX:105:ASN:OD1	1:QX:266:SER:OG	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GY:1587:GLU:HA	2:GY:1590:ILE:HD12	1.82	0.62
1:OX:282:VAL:HG13	1:OX:289:TYR:HB2	1.82	0.61
1:PX:73:GLU:OE2	1:PX:315:ARG:NH1	2.21	0.61
2:FY:1536:ALA:HB3	2:GY:1519:VAL:HG23	1.82	0.61
2:IY:1587:GLU:HA	2:IY:1590:ILE:HD12	1.81	0.61
1:AX:78:ILE:HG21	1:AX:90:PRO:HG3	1.82	0.61
1:CX:299:ASP:OD1	1:CX:299:ASP:N	2.30	0.61
1:HX:104:SER:HB2	2:GY:1547:PHE:HB3	1.82	0.61
1:FX:45:LYS:HD3	1:FX:309:LYS:HB3	1.83	0.61
1:GX:61:LEU:HD22	1:GX:271:PRO:HG2	1.83	0.61
1:AX:43:ASN:HD21	1:QX:52:GLU:HA	1.64	0.61
2:CY:1587:GLU:HA	2:CY:1590:ILE:HD12	1.81	0.61
1:GX:73:GLU:OE2	1:GX:315:ARG:NH1	2.21	0.61
1:QX:277:ARG:HD2	1:QX:294:ARG:HH11	1.66	0.61
2:NY:1536:ALA:HB3	2:OY:1519:VAL:HG23	1.81	0.61
2:HY:1470:SER:OG	2:HY:1471:LYS:N	2.34	0.61
1:DX:277:ARG:HD2	1:DX:294:ARG:HH11	1.66	0.61
1:LX:92:SER:O	1:LX:93:ASN:ND2	2.34	0.61
1:CX:45:LYS:HD3	1:CX:309:LYS:HB3	1.83	0.60
1:MX:61:LEU:HD12	2:LY:1527:ARG:HD3	1.83	0.60
1:PX:284:THR:HG23	1:PX:286:LYS:H	1.65	0.60
1:MX:299:ASP:OD1	1:MX:299:ASP:N	2.32	0.60
2:DY:1587:GLU:HA	2:DY:1590:ILE:HD12	1.82	0.60
1:MX:105:ASN:OD1	1:MX:266:SER:OG	2.18	0.60
1:HX:92:SER:O	1:HX:93:ASN:ND2	2.34	0.60
2:AY:1519:VAL:HG23	2:QY:1536:ALA:HB3	1.83	0.60
1:AX:120:ARG:NH1	1:QX:129:LYS:O	2.34	0.60
1:OX:73:GLU:OE2	1:OX:315:ARG:NH1	2.19	0.60
1:DX:51:ASP:O	1:EX:43:ASN:ND2	2.35	0.60
2:BY:1587:GLU:OE1	2:BY:1591:LYS:NZ	2.34	0.60
1:BX:282:VAL:HG13	1:BX:289:TYR:HB2	1.83	0.60
1:QX:61:LEU:HD22	1:QX:271:PRO:HG2	1.84	0.59
2:BY:1489:THR:O	2:BY:1491:GLN:NE2	2.34	0.59
2:MY:1533:ASP:HA	2:NY:1519:VAL:HG21	1.84	0.59
1:DX:92:SER:HB2	2:CY:1560:ASN:HA	1.85	0.59
1:GX:92:SER:O	1:GX:93:ASN:ND2	2.35	0.59
1:CX:77:TYR:HB2	1:CX:283:ARG:HH21	1.67	0.59
1:JX:299:ASP:HB2	2:JY:1512:ILE:HD13	1.84	0.59
2:JY:1587:GLU:HA	2:JY:1590:ILE:HD12	1.84	0.59
1:AX:45:LYS:HD3	1:AX:309:LYS:HB3	1.84	0.59
1:BX:288:LEU:HD22	1:CX:68:GLN:HE21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CX:277:ARG:HD2	1:CX:294:ARG:HH11	1.67	0.59
2:HY:1533:ASP:HA	2:IY:1519:VAL:HG21	1.85	0.59
1:LX:51:ASP:O	1:MX:43:ASN:ND2	2.35	0.59
2:LY:1587:GLU:HA	2:LY:1590:ILE:HD12	1.84	0.59
1:FX:73:GLU:OE2	1:FX:315:ARG:NH1	2.20	0.59
1:HX:36:ARG:HH11	2:GY:1488:PRO:HD3	1.67	0.59
1:BX:80:THR:HG22	1:BX:280:LEU:HD13	1.85	0.59
1:FX:80:THR:HG22	1:FX:280:LEU:HA	1.84	0.59
1:PX:61:LEU:HD22	1:PX:271:PRO:HG2	1.83	0.59
2:BY:1587:GLU:HA	2:BY:1590:ILE:HD12	1.83	0.59
2:DY:1482:LEU:HD13	2:DY:1513:LYS:HD2	1.85	0.59
1:LX:61:LEU:HD12	2:KY:1527:ARG:HD3	1.85	0.58
1:OX:62:ASP:OD2	2:MY:1548:LYS:NZ	2.36	0.58
2:AY:1489:THR:O	2:AY:1491:GLN:NE2	2.35	0.58
2:LY:1489:THR:O	2:LY:1491:GLN:NE2	2.36	0.58
1:EX:92:SER:O	1:EX:93:ASN:ND2	2.36	0.58
1:IX:61:LEU:HD22	1:IX:271:PRO:HG2	1.85	0.58
2:EY:1587:GLU:HA	2:EY:1590:ILE:HD12	1.84	0.58
1:DX:61:LEU:HD22	1:DX:271:PRO:HG2	1.84	0.58
2:AY:1470:SER:OG	2:AY:1471:LYS:N	2.35	0.58
2:AY:1587:GLU:HA	2:AY:1590:ILE:HD12	1.84	0.58
2:PY:1470:SER:OG	2:PY:1471:LYS:N	2.34	0.58
1:BX:67:ILE:HD11	1:BX:97:ILE:HD13	1.85	0.58
1:NX:284:THR:HG23	1:NX:286:LYS:H	1.68	0.58
1:PX:92:SER:O	1:PX:93:ASN:ND2	2.37	0.58
2:PY:1587:GLU:HA	2:PY:1590:ILE:HD12	1.85	0.58
1:AX:61:LEU:HD12	2:QY:1527:ARG:HD3	1.83	0.58
1:JX:288:LEU:HD22	1:KX:68:GLN:HE21	1.68	0.58
2:KY:1564:ASP:OD1	2:KY:1564:ASP:N	2.31	0.58
1:BX:280:LEU:N	1:BX:291:PHE:O	2.30	0.58
1:CX:92:SER:O	1:CX:93:ASN:ND2	2.36	0.58
1:EX:288:LEU:HD22	1:FX:68:GLN:HE21	1.68	0.58
1:FX:67:ILE:HD11	1:FX:97:ILE:HD13	1.86	0.58
1:LX:105:ASN:OD1	1:LX:266:SER:OG	2.19	0.58
1:EX:105:ASN:OD1	1:EX:266:SER:OG	2.21	0.58
1:IX:93:ASN:HD22	2:HY:1566:ILE:HD13	1.69	0.58
1:GX:105:ASN:OD1	1:GX:266:SER:OG	2.19	0.58
2:DY:1536:ALA:HB3	2:EY:1519:VAL:HG23	1.86	0.58
2:FY:1534:ASN:OD1	2:FY:1538:LYS:NZ	2.30	0.58
2:AY:1536:ALA:HB3	2:BY:1519:VAL:HG23	1.86	0.57
2:BY:1482:LEU:HD13	2:BY:1513:LYS:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GY:1503:ASP:OD2	2:GY:1504:SER:N	2.36	0.57
1:FX:105:ASN:OD1	1:FX:266:SER:OG	2.20	0.57
1:CX:105:ASN:OD1	1:CX:266:SER:OG	2.20	0.57
1:DX:77:TYR:HA	2:CY:1555:THR:HG23	1.85	0.57
1:JX:277:ARG:HD2	1:JX:294:ARG:NH1	2.19	0.57
1:JX:282:VAL:HG13	1:JX:289:TYR:HB2	1.86	0.57
1:MX:67:ILE:HA	1:MX:308:VAL:HG13	1.85	0.57
2:HY:1489:THR:O	2:HY:1491:GLN:NE2	2.36	0.57
1:CX:289:TYR:HH	1:CX:312:TYR:HH	1.53	0.57
1:BX:67:ILE:HA	1:BX:308:VAL:HG23	1.85	0.57
1:BX:92:SER:O	1:BX:93:ASN:ND2	2.37	0.57
1:FX:59:THR:OG1	1:FX:60:SER:N	2.37	0.57
1:KX:45:LYS:HD3	1:KX:309:LYS:HB3	1.86	0.57
1:DX:61:LEU:HD12	2:CY:1527:ARG:HD3	1.87	0.57
1:EX:71:LYS:HE2	2:DY:1566:ILE:HB	1.87	0.57
2:JY:1533:ASP:HA	2:KY:1519:VAL:HG21	1.86	0.57
2:QY:1587:GLU:HA	2:QY:1590:ILE:HD12	1.86	0.57
1:CX:62:ASP:OD1	2:AY:1548:LYS:NZ	2.37	0.57
1:NX:61:LEU:HD22	1:NX:271:PRO:HG2	1.87	0.57
2:CY:1533:ASP:HA	2:DY:1519:VAL:HG21	1.87	0.57
2:HY:1536:ALA:HB3	2:IY:1519:VAL:HG23	1.86	0.57
1:CX:101:SER:OG	2:AY:1549:ASN:ND2	2.38	0.57
1:OX:45:LYS:HD3	1:OX:309:LYS:HB3	1.87	0.57
1:HX:45:LYS:HD3	1:HX:309:LYS:HB3	1.87	0.56
1:HX:67:ILE:HA	1:HX:308:VAL:HG23	1.87	0.56
1:GX:59:THR:OG1	1:GX:60:SER:N	2.38	0.56
1:HX:77:TYR:HA	2:GY:1555:THR:HG23	1.86	0.56
1:QX:78:ILE:HG21	1:QX:90:PRO:HG3	1.86	0.56
1:AX:59:THR:HG21	1:AX:86:TRP:CZ3	2.40	0.56
1:CX:61:LEU:HD22	1:CX:271:PRO:HG2	1.86	0.56
1:AX:105:ASN:OD1	1:AX:266:SER:OG	2.20	0.56
1:QX:289:TYR:HH	1:QX:312:TYR:HH	1.53	0.56
2:NY:1482:LEU:HD13	2:NY:1513:LYS:HD2	1.87	0.56
1:JX:59:THR:OG1	1:JX:60:SER:N	2.38	0.56
1:OX:92:SER:O	1:OX:93:ASN:ND2	2.38	0.56
2:FY:1489:THR:O	2:FY:1491:GLN:NE2	2.39	0.56
2:MY:1543:LEU:HD12	2:NY:1526:LEU:HD11	1.87	0.56
1:AX:92:SER:O	1:AX:93:ASN:ND2	2.39	0.56
1:EX:78:ILE:HG21	1:EX:90:PRO:HG3	1.88	0.56
1:IX:271:PRO:HB3	1:IX:276:TRP:CE2	2.40	0.56
1:OX:57:ILE:HD12	1:OX:308:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BY:1503:ASP:OD2	2:BY:1504:SER:N	2.38	0.56
2:DY:1489:THR:O	2:DY:1491:GLN:NE2	2.39	0.56
1:CX:280:LEU:N	1:CX:291:PHE:O	2.36	0.56
1:PX:77:TYR:HB2	1:PX:283:ARG:HH21	1.71	0.56
2:NY:1533:ASP:HA	2:OY:1519:VAL:HG21	1.87	0.56
1:HX:80:THR:HG22	1:HX:280:LEU:HD13	1.88	0.56
1:PX:45:LYS:HD3	1:PX:309:LYS:HB3	1.88	0.56
1:DX:45:LYS:HD3	1:DX:309:LYS:HB3	1.87	0.56
1:DX:277:ARG:HD2	1:DX:294:ARG:NH1	2.20	0.56
1:EX:104:SER:HB2	2:DY:1547:PHE:HB3	1.88	0.56
1:KX:92:SER:O	1:KX:93:ASN:ND2	2.39	0.56
1:BX:284:THR:HG23	1:BX:286:LYS:H	1.71	0.56
2:LY:1503:ASP:OD2	2:LY:1504:SER:N	2.39	0.56
1:LX:45:LYS:HD3	1:LX:309:LYS:HB3	1.87	0.55
1:NX:289:TYR:OH	1:NX:312:TYR:OH	2.22	0.55
2:FY:1487:ASP:OD2	2:FY:1489:THR:OG1	2.21	0.55
1:MX:59:THR:OG1	1:MX:60:SER:N	2.40	0.55
1:OX:78:ILE:HG21	1:OX:90:PRO:HG3	1.87	0.55
1:CX:282:VAL:HG13	1:CX:289:TYR:HB2	1.88	0.55
1:HX:61:LEU:HD22	1:HX:271:PRO:HG2	1.88	0.55
1:LX:282:VAL:HG13	1:LX:289:TYR:HB2	1.87	0.55
2:LY:1495:GLU:OE2	2:LY:1506:ARG:NH2	2.39	0.55
1:EX:45:LYS:HD3	1:EX:309:LYS:HB3	1.87	0.55
1:GX:282:VAL:HG13	1:GX:289:TYR:HB2	1.88	0.55
2:GY:1579:ASP:HB3	2:GY:1582:LYS:HD3	1.88	0.55
1:IX:59:THR:OG1	1:IX:60:SER:N	2.40	0.55
2:GY:1470:SER:OG	2:GY:1471:LYS:N	2.40	0.55
2:KY:1489:THR:O	2:KY:1491:GLN:NE2	2.39	0.55
2:PY:1533:ASP:HA	2:QY:1519:VAL:HG21	1.88	0.55
1:GX:46:ILE:HG23	1:GX:310:LEU:HD23	1.88	0.55
1:JX:271:PRO:HA	1:JX:276:TRP:CZ3	2.42	0.55
1:MX:45:LYS:HD3	1:MX:309:LYS:HB3	1.88	0.55
1:NX:45:LYS:HD3	1:NX:309:LYS:HB3	1.89	0.55
1:AX:51:ASP:O	1:BX:43:ASN:ND2	2.39	0.55
1:KX:284:THR:OG1	1:KX:285:ASN:N	2.38	0.55
1:KX:288:LEU:HD22	1:LX:68:GLN:HE21	1.71	0.55
1:QX:282:VAL:HG13	1:QX:289:TYR:HB2	1.87	0.55
2:HY:1587:GLU:HA	2:HY:1590:ILE:HD12	1.88	0.55
2:OY:1587:GLU:HA	2:OY:1590:ILE:HD12	1.88	0.55
1:CX:73:GLU:HG2	1:CX:286:LYS:HB2	1.88	0.55
1:FX:62:ASP:OD1	2:DY:1548:LYS:NZ	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AX:94:HIS:NE2	1:QX:283:ARG:HD3	2.22	0.55
2:LY:1533:ASP:HA	2:MY:1519:VAL:HG21	1.88	0.55
1:CX:283:ARG:HD3	1:DX:94:HIS:NE2	2.22	0.54
1:JX:289:TYR:OH	1:JX:312:TYR:OH	2.23	0.54
1:MX:61:LEU:HD22	1:MX:271:PRO:HG2	1.87	0.54
2:QY:1482:LEU:HD13	2:QY:1513:LYS:HD2	1.89	0.54
1:GX:89:VAL:HG13	1:GX:96:PHE:HB2	1.88	0.54
1:NX:92:SER:O	1:NX:93:ASN:ND2	2.41	0.54
1:IX:282:VAL:HG13	1:IX:289:TYR:HB2	1.89	0.54
2:IY:1533:ASP:HA	2:JY:1519:VAL:HG21	1.88	0.54
2:JY:1495:GLU:OE2	2:JY:1506:ARG:NH2	2.41	0.54
2:MY:1587:GLU:HA	2:MY:1590:ILE:HD12	1.88	0.54
1:KX:105:ASN:OD1	1:KX:266:SER:OG	2.19	0.54
2:IY:1482:LEU:HD13	2:IY:1513:LYS:HD2	1.88	0.54
2:LY:1536:ALA:HB3	2:MY:1519:VAL:HG23	1.88	0.54
1:JX:48:TYR:HD1	1:JX:55:ILE:HD11	1.71	0.54
1:FX:284:THR:OG1	1:FX:285:ASN:N	2.39	0.54
1:MX:277:ARG:HD2	1:MX:294:ARG:HH11	1.72	0.54
1:QX:92:SER:HB2	2:PY:1560:ASN:HA	1.88	0.54
2:QY:1489:THR:O	2:QY:1491:GLN:NE2	2.40	0.54
1:JX:61:LEU:HD22	1:JX:271:PRO:HG2	1.90	0.54
2:GY:1482:LEU:HD13	2:GY:1513:LYS:HD2	1.89	0.54
1:EX:271:PRO:HB3	1:EX:276:TRP:CE2	2.43	0.54
1:KX:129:LYS:O	1:LX:120:ARG:NH1	2.41	0.54
1:OX:105:ASN:OD1	1:OX:266:SER:OG	2.20	0.54
1:PX:282:VAL:HG13	1:PX:289:TYR:HB2	1.89	0.54
2:NY:1587:GLU:HA	2:NY:1590:ILE:HD12	1.89	0.54
1:BX:45:LYS:HD3	1:BX:309:LYS:HB3	1.90	0.53
1:CX:67:ILE:HA	1:CX:308:VAL:HG23	1.88	0.53
1:GX:284:THR:OG1	1:GX:285:ASN:N	2.40	0.53
1:KX:61:LEU:HD22	1:KX:271:PRO:HG2	1.90	0.53
2:IY:1536:ALA:HB3	2:JY:1519:VAL:HG23	1.90	0.53
1:EX:51:ASP:O	1:FX:43:ASN:ND2	2.41	0.53
1:GX:299:ASP:OD1	1:GX:299:ASP:N	2.31	0.53
2:FY:1587:GLU:HA	2:FY:1590:ILE:HD12	1.90	0.53
1:IX:283:ARG:HD3	1:JX:94:HIS:NE2	2.23	0.53
1:JX:37:GLY:HA2	1:JX:298:LYS:HB2	1.91	0.53
1:HX:271:PRO:HB3	1:HX:276:TRP:CE2	2.43	0.53
1:LX:277:ARG:HD2	1:LX:294:ARG:NH1	2.24	0.53
1:NX:43:ASN:OD1	1:NX:43:ASN:N	2.38	0.53
2:GY:1587:GLU:OE1	2:GY:1591:LYS:NZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AY:1519:VAL:HG21	2:QY:1533:ASP:HA	1.91	0.53
2:KY:1536:ALA:HB3	2:LY:1519:VAL:HG23	1.91	0.53
1:BX:59:THR:OG1	1:BX:60:SER:N	2.41	0.53
2:GY:1579:ASP:OD1	2:GY:1582:LYS:N	2.34	0.53
1:BX:68:GLN:HE22	1:BX:94:HIS:CD2	2.27	0.53
1:NX:282:VAL:HG13	1:NX:289:TYR:HB2	1.91	0.53
1:PX:59:THR:OG1	1:PX:60:SER:N	2.41	0.53
1:QX:45:LYS:HD3	1:QX:309:LYS:HB3	1.90	0.53
2:CY:1596:GLU:HA	2:CY:1599:LEU:HD23	1.91	0.53
2:GY:1536:ALA:HB3	2:HY:1519:VAL:HG23	1.90	0.53
1:EX:39:VAL:HG11	1:EX:60:SER:HB2	1.91	0.53
2:JY:1470:SER:OG	2:JY:1471:LYS:N	2.42	0.53
2:PY:1585:GLU:O	2:PY:1589:THR:HG23	2.09	0.53
1:AX:59:THR:OG1	1:AX:60:SER:N	2.41	0.52
1:CX:58:TRP:H	1:CX:305:TYR:HD2	1.57	0.52
1:DX:271:PRO:HB3	1:DX:276:TRP:CE2	2.42	0.52
1:LX:68:GLN:HA	1:LX:94:HIS:HB3	1.90	0.52
1:BX:129:LYS:O	1:CX:120:ARG:NH1	2.42	0.52
1:GX:57:ILE:HD12	1:GX:308:VAL:HG21	1.91	0.52
1:GX:67:ILE:HA	1:GX:308:VAL:HG23	1.92	0.52
1:IX:45:LYS:HD3	1:IX:309:LYS:HB3	1.91	0.52
1:IX:68:GLN:HE22	1:IX:94:HIS:CD2	2.27	0.52
1:LX:80:THR:HG22	1:LX:280:LEU:HD13	1.92	0.52
1:OX:59:THR:OG1	1:OX:60:SER:N	2.41	0.52
2:KY:1470:SER:OG	2:KY:1471:LYS:N	2.40	0.52
1:EX:282:VAL:HG13	1:EX:289:TYR:HB2	1.92	0.52
1:GX:67:ILE:HD11	1:GX:97:ILE:HD13	1.91	0.52
1:GX:71:LYS:HE2	2:FY:1566:ILE:HB	1.91	0.52
1:KX:59:THR:OG1	1:KX:60:SER:N	2.42	0.52
2:HY:1503:ASP:OD1	2:HY:1504:SER:N	2.42	0.52
2:JY:1503:ASP:OD2	2:JY:1504:SER:N	2.42	0.52
1:DX:283:ARG:HD3	1:EX:94:HIS:NE2	2.25	0.52
1:GX:277:ARG:HD2	1:GX:294:ARG:HH11	1.74	0.52
1:JX:129:LYS:O	1:KX:120:ARG:NH1	2.42	0.52
2:DY:1503:ASP:OD1	2:DY:1504:SER:N	2.43	0.52
2:GY:1489:THR:O	2:GY:1491:GLN:NE2	2.42	0.52
1:FX:73:GLU:HG2	1:FX:286:LYS:HB2	1.92	0.52
1:BX:78:ILE:HG21	1:BX:90:PRO:HG3	1.91	0.52
2:EY:1489:THR:O	2:EY:1491:GLN:NE2	2.41	0.52
2:MY:1487:ASP:OD1	2:MY:1489:THR:OG1	2.24	0.52
1:AX:282:VAL:HG13	1:AX:289:TYR:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:FX:89:VAL:HG13	1:FX:96:PHE:HB2	1.90	0.52
1:FX:101:SER:OG	2:DY:1549:ASN:ND2	2.42	0.52
1:GX:45:LYS:HD3	1:GX:309:LYS:HB3	1.91	0.52
1:HX:59:THR:OG1	1:HX:60:SER:N	2.43	0.52
1:PX:36:ARG:HG2	1:PX:38:ARG:H	1.75	0.52
2:IY:1470:SER:OG	2:IY:1471:LYS:N	2.43	0.52
2:NY:1503:ASP:OD2	2:NY:1504:SER:N	2.43	0.52
1:CX:61:LEU:HD12	2:BY:1527:ARG:HD3	1.91	0.52
1:QX:68:GLN:HG2	1:QX:309:LYS:HG3	1.91	0.52
2:BY:1536:ALA:HB3	2:CY:1519:VAL:HG23	1.91	0.52
2:OY:1470:SER:OG	2:OY:1471:LYS:N	2.41	0.52
2:QY:1577:GLU:HG2	2:QY:1578:PRO:O	2.10	0.52
1:GX:78:ILE:HG21	1:GX:90:PRO:HG3	1.91	0.52
2:AY:1577:GLU:HG2	2:AY:1578:PRO:O	2.10	0.52
2:EY:1495:GLU:OE2	2:EY:1506:ARG:NH2	2.42	0.52
2:EY:1585:GLU:O	2:EY:1589:THR:HG23	2.10	0.52
1:AX:61:LEU:HD22	1:AX:271:PRO:HG2	1.91	0.52
1:DX:68:GLN:HB3	1:DX:309:LYS:HA	1.92	0.52
1:DX:282:VAL:HG13	1:DX:289:TYR:HB2	1.90	0.52
1:PX:289:TYR:HH	1:PX:312:TYR:HH	1.54	0.52
2:CY:1585:GLU:O	2:CY:1589:THR:HG23	2.10	0.52
2:EY:1470:SER:OG	2:EY:1471:LYS:N	2.43	0.52
2:FY:1482:LEU:HD13	2:FY:1513:LYS:HD2	1.91	0.52
1:CX:92:SER:HB2	2:BY:1560:ASN:HA	1.92	0.51
1:FX:93:ASN:HD22	2:EY:1566:ILE:HD13	1.75	0.51
1:NX:59:THR:OG1	1:NX:60:SER:N	2.43	0.51
2:AY:1585:GLU:O	2:AY:1589:THR:HG23	2.10	0.51
2:LY:1585:GLU:O	2:LY:1589:THR:HG23	2.11	0.51
1:GX:48:TYR:HB2	1:GX:310:LEU:HD22	1.93	0.51
1:NX:80:THR:HG22	1:NX:280:LEU:HD13	1.92	0.51
1:QX:271:PRO:HB3	1:QX:276:TRP:CE2	2.44	0.51
2:EY:1564:ASP:OD1	2:EY:1564:ASP:N	2.44	0.51
2:IY:1585:GLU:O	2:IY:1589:THR:HG23	2.10	0.51
1:AX:77:TYR:HA	2:QY:1555:THR:HG23	1.92	0.51
1:DX:67:ILE:HA	1:DX:308:VAL:HG23	1.90	0.51
1:FX:88:ILE:HG12	1:FX:97:ILE:HG22	1.93	0.51
1:IX:61:LEU:HD12	2:HY:1527:ARG:HD3	1.93	0.51
1:NX:60:SER:OG	1:NX:63:ASN:ND2	2.43	0.51
1:PX:71:LYS:HE2	2:OY:1566:ILE:HB	1.91	0.51
2:AY:1587:GLU:OE2	2:AY:1591:LYS:NZ	2.43	0.51
2:BY:1470:SER:OG	2:BY:1471:LYS:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:OY:1585:GLU:O	2:OY:1589:THR:HG23	2.10	0.51
1:DX:67:ILE:HD11	1:DX:97:ILE:HD13	1.92	0.51
1:EX:59:THR:OG1	1:EX:60:SER:N	2.43	0.51
1:GX:68:GLN:HE22	1:GX:94:HIS:CD2	2.28	0.51
1:LX:299:ASP:OD1	1:LX:299:ASP:N	2.33	0.51
2:FY:1503:ASP:OD2	2:FY:1504:SER:N	2.43	0.51
2:MY:1535:MET:HE2	2:MY:1544:PRO:HD3	1.91	0.51
1:NX:68:GLN:HA	1:NX:94:HIS:HB3	1.92	0.51
2:OY:1577:GLU:HG2	2:OY:1578:PRO:O	2.10	0.51
2:PY:1577:GLU:HG2	2:PY:1578:PRO:O	2.11	0.51
2:PY:1586:THR:HG22	2:QY:1599:LEU:HB2	1.92	0.51
2:QY:1585:GLU:O	2:QY:1589:THR:HG23	2.11	0.51
1:MX:68:GLN:HG2	1:MX:309:LYS:HG3	1.93	0.51
1:HX:33:ASN:OD1	1:HX:34:PHE:N	2.43	0.51
1:JX:284:THR:OG1	1:JX:285:ASN:N	2.42	0.51
1:MX:92:SER:O	1:MX:93:ASN:ND2	2.44	0.51
1:MX:282:VAL:HG13	1:MX:289:TYR:HB2	1.92	0.51
1:QX:68:GLN:HB3	1:QX:309:LYS:HA	1.92	0.51
2:HY:1534:ASN:OD1	2:HY:1538:LYS:NZ	2.31	0.51
2:NY:1534:ASN:OD1	2:NY:1538:LYS:NZ	2.31	0.51
1:JX:289:TYR:O	1:JX:290:GLN:NE2	2.44	0.51
1:LX:59:THR:OG1	1:LX:60:SER:N	2.42	0.51
2:FY:1585:GLU:O	2:FY:1589:THR:HG23	2.11	0.51
2:KY:1585:GLU:O	2:KY:1589:THR:HG23	2.10	0.51
2:MY:1593:LYS:HD2	2:NY:1603:LEU:HA	1.93	0.51
1:AX:59:THR:HG21	1:AX:86:TRP:HZ3	1.75	0.50
1:MX:73:GLU:HG2	1:MX:286:LYS:HB2	1.92	0.50
1:NX:277:ARG:HD2	1:NX:294:ARG:NH1	2.25	0.50
1:OX:68:GLN:HA	1:OX:94:HIS:HB3	1.93	0.50
2:DY:1585:GLU:O	2:DY:1589:THR:HG23	2.11	0.50
1:DX:57:ILE:HD12	1:DX:308:VAL:HG21	1.92	0.50
1:EX:62:ASP:OD1	2:CY:1548:LYS:NZ	2.44	0.50
1:QX:73:GLU:HG2	1:QX:286:LYS:HB2	1.93	0.50
2:BY:1585:GLU:O	2:BY:1589:THR:HG23	2.11	0.50
2:CY:1577:GLU:HG2	2:CY:1578:PRO:O	2.11	0.50
2:GY:1577:GLU:HG2	2:GY:1578:PRO:O	2.12	0.50
1:JX:68:GLN:HA	1:JX:94:HIS:HB3	1.94	0.50
1:LX:271:PRO:HB3	1:LX:276:TRP:CE2	2.47	0.50
1:MX:43:ASN:OD1	1:MX:43:ASN:N	2.42	0.50
1:PX:283:ARG:HD3	1:QX:94:HIS:NE2	2.26	0.50
1:QX:93:ASN:HD22	2:PY:1566:ILE:HD13	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CY:1576:ILE:HG21	2:DY:1584:TYR:CE1	2.45	0.50
2:DY:1577:GLU:HG2	2:DY:1578:PRO:O	2.12	0.50
1:IX:299:ASP:OD1	1:IX:299:ASP:N	2.32	0.50
1:JX:61:LEU:HD12	2:IY:1527:ARG:HD3	1.93	0.50
1:JX:105:ASN:OD1	1:JX:266:SER:OG	2.22	0.50
1:NX:129:LYS:O	1:OX:120:ARG:NH1	2.44	0.50
1:AX:68:GLN:HA	1:AX:94:HIS:HB3	1.93	0.50
1:DX:33:ASN:OD1	1:DX:34:PHE:N	2.44	0.50
1:GX:289:TYR:OH	1:GX:312:TYR:OH	2.24	0.50
1:IX:277:ARG:HD2	1:IX:294:ARG:HH11	1.75	0.50
2:EY:1503:ASP:OD1	2:EY:1504:SER:N	2.44	0.50
2:GY:1514:ARG:HG3	2:GY:1515:GLN:N	2.26	0.50
1:JX:289:TYR:HH	1:JX:312:TYR:HH	1.56	0.50
1:OX:71:LYS:HE2	2:NY:1566:ILE:HB	1.94	0.50
2:IY:1576:ILE:HG21	2:JY:1584:TYR:CE1	2.42	0.50
1:LX:73:GLU:HG2	1:LX:286:LYS:HB2	1.92	0.50
1:QX:92:SER:O	1:QX:93:ASN:ND2	2.45	0.50
2:OY:1533:ASP:HA	2:PY:1519:VAL:HG21	1.94	0.50
1:CX:290:GLN:NE2	1:DX:307:THR:OG1	2.45	0.50
2:CY:1503:ASP:OD1	2:CY:1504:SER:N	2.45	0.50
2:GY:1533:ASP:HA	2:HY:1519:VAL:HG21	1.94	0.50
2:IY:1564:ASP:OD1	2:IY:1564:ASP:N	2.33	0.50
2:NY:1585:GLU:O	2:NY:1589:THR:HG23	2.12	0.50
2:OY:1489:THR:O	2:OY:1491:GLN:NE2	2.42	0.50
1:EX:305:TYR:HB3	1:EX:308:VAL:HG13	1.94	0.50
2:HY:1585:GLU:O	2:HY:1589:THR:HG23	2.12	0.50
1:CX:271:PRO:HB3	1:CX:276:TRP:CE2	2.47	0.49
1:HX:277:ARG:HD2	1:HX:294:ARG:NH1	2.24	0.49
1:JX:280:LEU:N	1:JX:291:PHE:O	2.45	0.49
2:AY:1593:LYS:HD2	2:BY:1603:LEU:HD23	1.94	0.49
2:NY:1577:GLU:HG2	2:NY:1578:PRO:O	2.12	0.49
1:FX:282:VAL:HG13	1:FX:289:TYR:HB2	1.93	0.49
1:JX:92:SER:O	1:JX:93:ASN:ND2	2.45	0.49
2:BY:1577:GLU:HG2	2:BY:1578:PRO:O	2.12	0.49
2:JY:1536:ALA:HB3	2:KY:1519:VAL:HG23	1.93	0.49
2:JY:1577:GLU:HG2	2:JY:1578:PRO:O	2.12	0.49
2:JY:1585:GLU:O	2:JY:1589:THR:HG23	2.11	0.49
2:MY:1482:LEU:HD13	2:MY:1513:LYS:HD2	1.94	0.49
1:DX:78:ILE:HG21	1:DX:90:PRO:HG3	1.93	0.49
1:EX:284:THR:HG23	1:EX:286:LYS:H	1.77	0.49
1:HX:105:ASN:OD1	1:HX:266:SER:OG	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AX:271:PRO:HB3	1:AX:276:TRP:CE2	2.48	0.49
1:HX:282:VAL:HG13	1:HX:289:TYR:HB2	1.94	0.49
1:MX:278:THR:OG1	1:MX:279:ASN:N	2.46	0.49
2:EY:1536:ALA:HB3	2:FY:1519:VAL:HG23	1.95	0.49
2:JY:1486:ASP:OD1	2:JY:1487:ASP:N	2.45	0.49
2:MY:1577:GLU:HG2	2:MY:1578:PRO:O	2.13	0.49
1:CX:277:ARG:HD2	1:CX:294:ARG:NH1	2.27	0.49
1:GX:59:THR:HG21	1:GX:86:TRP:CZ3	2.47	0.49
1:HX:121:ASP:HA	1:HX:124:GLU:HG3	1.94	0.49
1:PX:68:GLN:HA	1:PX:94:HIS:HB3	1.94	0.49
1:PX:101:SER:OG	2:NY:1549:ASN:ND2	2.45	0.49
1:CX:57:ILE:HG21	1:CX:97:ILE:HD11	1.94	0.49
1:DX:92:SER:O	1:DX:93:ASN:ND2	2.45	0.49
1:GX:283:ARG:HD3	1:HX:94:HIS:NE2	2.28	0.49
1:HX:57:ILE:HD12	1:HX:308:VAL:HG21	1.95	0.49
2:DY:1534:ASN:OD1	2:DY:1538:LYS:NZ	2.32	0.49
1:DX:80:THR:HG22	1:DX:280:LEU:HD13	1.95	0.49
1:FX:36:ARG:HH11	2:EY:1488:PRO:HD3	1.78	0.49
1:IX:105:ASN:OD1	1:IX:266:SER:OG	2.22	0.49
1:PX:106:LEU:HD21	1:PX:267:ILE:HD13	1.94	0.49
2:GY:1585:GLU:O	2:GY:1589:THR:HG23	2.11	0.49
2:HY:1577:GLU:HG2	2:HY:1578:PRO:O	2.12	0.49
1:EX:67:ILE:HD11	1:EX:97:ILE:HD13	1.94	0.49
1:HX:59:THR:HG21	1:HX:86:TRP:CZ3	2.48	0.49
1:NX:59:THR:HG21	1:NX:86:TRP:CZ3	2.48	0.49
2:EY:1533:ASP:HA	2:FY:1519:VAL:HG21	1.94	0.49
2:JY:1535:MET:HE2	2:JY:1544:PRO:HD3	1.95	0.49
2:KY:1479:SER:HB2	2:KY:1509:ILE:HD11	1.94	0.49
2:KY:1482:LEU:HD13	2:KY:1513:LYS:HD2	1.95	0.49
2:MY:1536:ALA:HB3	2:NY:1519:VAL:HG23	1.95	0.49
1:MX:68:GLN:HA	1:MX:94:HIS:HB3	1.94	0.49
2:FY:1577:GLU:HG2	2:FY:1578:PRO:O	2.13	0.49
2:KY:1503:ASP:OD1	2:KY:1504:SER:N	2.45	0.49
2:MY:1503:ASP:OD1	2:MY:1504:SER:N	2.46	0.49
2:MY:1585:GLU:O	2:MY:1589:THR:HG23	2.12	0.49
1:AX:280:LEU:N	1:AX:291:PHE:O	2.41	0.49
1:CX:281:VAL:HG12	1:CX:290:GLN:HE22	1.76	0.49
1:MX:284:THR:HG23	1:MX:286:LYS:H	1.77	0.49
1:PX:271:PRO:HB3	1:PX:276:TRP:CE2	2.48	0.49
1:HX:67:ILE:HD11	1:HX:97:ILE:HD13	1.94	0.48
2:BY:1535:MET:HE2	2:BY:1544:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IY:1577:GLU:HG2	2:IY:1578:PRO:O	2.12	0.48
1:IX:262:PRO:HB2	2:HY:1542:LEU:HD11	1.93	0.48
2:AY:1503:ASP:OD2	2:AY:1504:SER:N	2.46	0.48
2:LY:1577:GLU:HG2	2:LY:1578:PRO:O	2.13	0.48
1:KX:78:ILE:HG21	1:KX:90:PRO:HG3	1.93	0.48
1:MX:59:THR:HG21	1:MX:86:TRP:CZ3	2.48	0.48
1:OX:45:LYS:HE3	1:OX:309:LYS:HD3	1.96	0.48
1:OX:68:GLN:HG2	1:OX:309:LYS:HG3	1.96	0.48
1:OX:289:TYR:OH	1:OX:312:TYR:OH	2.30	0.48
2:IY:1593:LYS:HD2	2:JY:1603:LEU:HA	1.94	0.48
2:PY:1482:LEU:HD13	2:PY:1513:LYS:HD2	1.96	0.48
1:DX:59:THR:HG21	1:DX:86:TRP:CZ3	2.47	0.48
2:BY:1495:GLU:OE2	2:BY:1506:ARG:NH2	2.46	0.48
2:NY:1499:GLU:OE1	2:NY:1500:GLY:N	2.46	0.48
1:CX:103:LYS:NZ	1:CX:268:GLU:HB3	2.29	0.48
1:DX:121:ASP:O	1:DX:124:GLU:HG3	2.13	0.48
1:GX:271:PRO:HA	1:GX:276:TRP:CZ3	2.49	0.48
1:OX:48:TYR:HD1	1:OX:55:ILE:HD11	1.78	0.48
2:JY:1499:GLU:OE1	2:JY:1500:GLY:N	2.46	0.48
2:QY:1503:ASP:OD2	2:QY:1504:SER:N	2.47	0.48
1:FX:67:ILE:HA	1:FX:308:VAL:HG23	1.95	0.48
1:QX:276:TRP:O	1:QX:278:THR:HG22	2.14	0.48
1:AX:299:ASP:OD1	1:AX:299:ASP:N	2.35	0.48
1:BX:61:LEU:HD22	1:BX:271:PRO:HG2	1.95	0.48
1:CX:59:THR:OG1	1:CX:60:SER:N	2.45	0.48
1:KX:271:PRO:HB3	1:KX:276:TRP:CE2	2.48	0.48
2:AY:1534:ASN:OD1	2:AY:1538:LYS:NZ	2.34	0.48
2:HY:1535:MET:HE2	2:HY:1544:PRO:HD3	1.95	0.48
2:KY:1495:GLU:OE2	2:KY:1506:ARG:NH2	2.47	0.48
2:OY:1503:ASP:OD1	2:OY:1504:SER:N	2.47	0.48
2:PY:1593:LYS:HD2	2:QY:1603:LEU:HD23	1.96	0.48
1:DX:299:ASP:OD1	1:DX:299:ASP:N	2.29	0.48
1:GX:276:TRP:O	1:GX:278:THR:HG22	2.14	0.48
1:IX:33:ASN:OD1	1:IX:34:PHE:N	2.46	0.48
1:LX:91:ASN:ND2	2:KY:1559:THR:OG1	2.46	0.48
1:OX:89:VAL:HG13	1:OX:96:PHE:HB2	1.95	0.48
1:OX:271:PRO:HB3	1:OX:276:TRP:CE2	2.49	0.48
2:KY:1577:GLU:HG2	2:KY:1578:PRO:O	2.13	0.48
1:EX:67:ILE:HA	1:EX:308:VAL:HG23	1.94	0.48
1:EX:88:ILE:HG12	1:EX:97:ILE:HG22	1.95	0.48
1:FX:276:TRP:O	1:FX:278:THR:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LX:59:THR:HG21	1:LX:86:TRP:CZ3	2.49	0.48
1:NX:280:LEU:N	1:NX:291:PHE:O	2.34	0.48
2:BY:1598:LYS:HA	2:BY:1601:LYS:HE3	1.95	0.48
1:DX:89:VAL:HG13	1:DX:96:PHE:HB2	1.95	0.47
1:IX:57:ILE:HD12	1:IX:308:VAL:HG11	1.96	0.47
1:JX:43:ASN:OD1	1:JX:43:ASN:N	2.34	0.47
1:QX:57:ILE:HD12	1:QX:308:VAL:HG21	1.96	0.47
1:QX:121:ASP:HA	1:QX:124:GLU:HG3	1.96	0.47
2:HY:1486:ASP:OD1	2:HY:1487:ASP:N	2.47	0.47
1:EX:68:GLN:HA	1:EX:94:HIS:HB3	1.94	0.47
1:NX:61:LEU:HD12	2:MY:1527:ARG:HD3	1.95	0.47
1:QX:80:THR:HG22	1:QX:280:LEU:HD13	1.94	0.47
2:MY:1564:ASP:OD1	2:MY:1564:ASP:N	2.45	0.47
2:QY:1495:GLU:OE2	2:QY:1506:ARG:NH2	2.47	0.47
1:AX:121:ASP:O	1:AX:124:GLU:HG3	2.14	0.47
1:CX:57:ILE:HD12	1:CX:308:VAL:HG21	1.95	0.47
1:HX:284:THR:OG1	1:HX:285:ASN:N	2.47	0.47
2:CY:1598:LYS:HA	2:CY:1601:LYS:HZ2	1.78	0.47
2:EY:1577:GLU:HG2	2:EY:1578:PRO:O	2.15	0.47
1:JX:57:ILE:HG21	1:JX:97:ILE:HD11	1.96	0.47
1:LX:301:PHE:O	2:LY:1476:HIS:HB2	2.14	0.47
2:EY:1514:ARG:O	2:EY:1518:GLU:HG2	2.15	0.47
2:IY:1503:ASP:OD2	2:IY:1504:SER:N	2.48	0.47
1:CX:276:TRP:O	1:CX:278:THR:HG22	2.15	0.47
1:FX:271:PRO:HB3	1:FX:276:TRP:CE2	2.50	0.47
1:KX:57:ILE:HD12	1:KX:308:VAL:HG21	1.95	0.47
1:QX:59:THR:HG21	1:QX:86:TRP:CZ3	2.49	0.47
2:NY:1470:SER:OG	2:NY:1471:LYS:N	2.45	0.47
1:BX:271:PRO:HA	1:BX:276:TRP:CZ3	2.50	0.47
1:LX:125:PHE:HA	1:LX:128:THR:HG22	1.97	0.47
1:AX:62:ASP:N	1:AX:62:ASP:OD2	2.47	0.47
1:DX:59:THR:OG1	1:DX:60:SER:N	2.47	0.47
1:GX:70:GLU:OE1	1:GX:315:ARG:NH1	2.46	0.47
1:KX:89:VAL:HG13	1:KX:96:PHE:HB2	1.96	0.47
1:OX:33:ASN:OD1	1:OX:34:PHE:N	2.48	0.47
2:EY:1534:ASN:OD1	2:EY:1538:LYS:NZ	2.34	0.47
2:KY:1487:ASP:OD2	2:KY:1489:THR:OG1	2.32	0.47
2:OY:1514:ARG:O	2:OY:1518:GLU:HG2	2.15	0.47
2:PY:1514:ARG:O	2:PY:1518:GLU:HG2	2.15	0.47
2:QY:1514:ARG:O	2:QY:1518:GLU:HG2	2.15	0.47
1:BX:33:ASN:OD1	1:BX:34:PHE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CX:281:VAL:HG12	1:CX:290:GLN:NE2	2.30	0.47
1:DX:301:PHE:O	2:DY:1476:HIS:HB2	2.15	0.47
1:GX:103:LYS:NZ	1:GX:268:GLU:HB3	2.29	0.47
1:JX:284:THR:HG23	1:JX:287:ALA:H	1.79	0.47
1:KX:276:TRP:O	1:KX:278:THR:HG22	2.15	0.47
1:NX:58:TRP:H	1:NX:305:TYR:HD2	1.62	0.47
1:OX:276:TRP:O	1:OX:278:THR:HG22	2.14	0.47
1:QX:305:TYR:HB3	1:QX:308:VAL:HG13	1.96	0.47
2:PY:1536:ALA:HB3	2:QY:1519:VAL:HG23	1.97	0.47
1:HX:68:GLN:HG2	1:HX:309:LYS:HG3	1.97	0.47
1:JX:305:TYR:HB3	1:JX:308:VAL:HG23	1.97	0.47
1:MX:44:LYS:HD3	1:MX:46:ILE:HG12	1.96	0.47
1:NX:73:GLU:O	1:NX:93:ASN:HA	2.15	0.47
1:BX:277:ARG:HH11	1:BX:294:ARG:NH1	2.13	0.47
1:GX:277:ARG:HD2	1:GX:294:ARG:NH1	2.29	0.47
1:HX:106:LEU:HD21	1:HX:267:ILE:HD13	1.97	0.47
1:MX:51:ASP:O	1:NX:43:ASN:ND2	2.48	0.47
1:MX:101:SER:OG	2:KY:1549:ASN:ND2	2.47	0.47
1:BX:277:ARG:HD2	1:BX:294:ARG:NH1	2.27	0.46
1:CX:68:GLN:HE22	1:CX:94:HIS:CD2	2.33	0.46
1:CX:88:ILE:HG12	1:CX:97:ILE:HG22	1.96	0.46
1:GX:78:ILE:HD13	1:GX:90:PRO:HB3	1.97	0.46
1:KX:277:ARG:HH11	1:KX:294:ARG:NH1	2.12	0.46
1:CX:68:GLN:HB3	1:CX:309:LYS:HA	1.97	0.46
1:NX:36:ARG:NH1	2:MY:1485:LEU:O	2.36	0.46
2:MY:1489:THR:O	2:MY:1491:GLN:NE2	2.45	0.46
1:HX:276:TRP:O	1:HX:278:THR:HG22	2.15	0.46
1:KX:59:THR:HG21	1:KX:86:TRP:CZ3	2.50	0.46
1:OX:77:TYR:HA	2:NY:1555:THR:HG23	1.98	0.46
1:OX:103:LYS:NZ	1:OX:268:GLU:HB3	2.31	0.46
1:OX:121:ASP:O	1:OX:124:GLU:HG3	2.16	0.46
2:AY:1576:ILE:HD13	2:BY:1584:TYR:CE1	2.50	0.46
1:EX:61:LEU:HD22	1:EX:271:PRO:HG2	1.98	0.46
1:GX:271:PRO:HB3	1:GX:276:TRP:CE2	2.50	0.46
1:IX:276:TRP:O	1:IX:278:THR:HG22	2.16	0.46
1:PX:280:LEU:N	1:PX:291:PHE:O	2.29	0.46
2:LY:1487:ASP:OD1	2:LY:1489:THR:OG1	2.31	0.46
1:AX:120:ARG:HH22	1:QX:130:LYS:HA	1.80	0.46
1:CX:36:ARG:NH1	2:BY:1485:LEU:O	2.40	0.46
1:FX:73:GLU:CD	1:FX:289:TYR:HH	2.17	0.46
2:BY:1593:LYS:HE3	2:BY:1593:LYS:HB3	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DX:280:LEU:N	1:DX:291:PHE:O	2.37	0.46
1:EX:59:THR:HG21	1:EX:86:TRP:CZ3	2.50	0.46
1:QX:46:ILE:HG21	1:QX:55:ILE:HG21	1.98	0.46
1:QX:77:TYR:HA	2:PY:1555:THR:HG23	1.97	0.46
2:DY:1533:ASP:HA	2:EY:1519:VAL:HG21	1.97	0.46
2:LY:1514:ARG:O	2:LY:1518:GLU:HG2	2.16	0.46
2:NY:1487:ASP:OD1	2:NY:1489:THR:OG1	2.32	0.46
1:KX:305:TYR:HB3	1:KX:308:VAL:HG13	1.96	0.46
1:MX:62:ASP:OD1	1:MX:62:ASP:N	2.49	0.46
1:MX:271:PRO:HB3	1:MX:276:TRP:CE2	2.51	0.46
1:NX:289:TYR:HH	1:NX:312:TYR:HH	1.48	0.46
2:LY:1564:ASP:OD1	2:LY:1564:ASP:N	2.42	0.46
2:PY:1503:ASP:OD2	2:PY:1504:SER:N	2.49	0.46
1:AX:73:GLU:HG2	1:AX:286:LYS:HB2	1.96	0.46
1:EX:68:GLN:HB3	1:EX:309:LYS:HA	1.98	0.46
1:FX:59:THR:HG21	1:FX:86:TRP:CZ3	2.50	0.46
1:HX:101:SER:OG	2:FY:1549:ASN:ND2	2.48	0.46
2:NY:1475:LEU:HD22	2:NY:1509:ILE:HD11	1.98	0.46
1:HX:68:GLN:HB3	1:HX:309:LYS:HA	1.97	0.46
1:QX:299:ASP:OD1	1:QX:299:ASP:N	2.33	0.46
2:JY:1534:ASN:OD1	2:JY:1538:LYS:NZ	2.35	0.46
2:NY:1593:LYS:HD2	2:OY:1603:LEU:HD23	1.98	0.46
2:PY:1486:ASP:OD2	2:PY:1487:ASP:N	2.49	0.46
1:BX:283:ARG:HD3	1:CX:94:HIS:NE2	2.31	0.45
1:JX:101:SER:OG	2:HY:1549:ASN:ND2	2.48	0.45
2:KY:1528:ASN:O	2:KY:1531:THR:OG1	2.26	0.45
1:GX:301:PHE:O	2:GY:1476:HIS:HB2	2.16	0.45
1:NX:271:PRO:HA	1:NX:276:TRP:CH2	2.52	0.45
1:PX:121:ASP:O	1:PX:124:GLU:HG3	2.16	0.45
1:PX:289:TYR:OH	1:PX:312:TYR:OH	2.24	0.45
2:AY:1486:ASP:OD1	2:AY:1487:ASP:N	2.49	0.45
1:AX:102:VAL:HG12	1:AX:103:LYS:N	2.31	0.45
1:AX:277:ARG:HH11	1:AX:294:ARG:NH1	2.14	0.45
1:BX:121:ASP:O	1:BX:124:GLU:HG3	2.16	0.45
1:FX:77:TYR:HA	2:EY:1555:THR:HG23	1.96	0.45
1:FX:121:ASP:O	1:FX:124:GLU:HG3	2.15	0.45
1:HX:299:ASP:OD1	1:HX:299:ASP:N	2.31	0.45
1:IX:267:ILE:HG13	1:IX:268:GLU:O	2.17	0.45
1:GX:66:VAL:O	1:GX:307:THR:HA	2.17	0.45
1:IX:88:ILE:HG23	1:IX:97:ILE:HG22	1.99	0.45
1:NX:77:TYR:HA	2:MY:1555:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:NX:301:PHE:O	2:NY:1476:HIS:HB2	2.16	0.45
1:OX:277:ARG:HH11	1:OX:294:ARG:NH1	2.14	0.45
2:IY:1486:ASP:OD1	2:IY:1487:ASP:N	2.49	0.45
2:IY:1495:GLU:OE2	2:IY:1506:ARG:NH2	2.49	0.45
1:AX:58:TRP:HH2	1:AX:294:ARG:HH21	1.64	0.45
1:AX:67:ILE:HD11	1:AX:97:ILE:HD13	1.97	0.45
1:FX:57:ILE:HD12	1:FX:308:VAL:HG21	1.98	0.45
1:JX:45:LYS:HE3	1:JX:309:LYS:HD3	1.98	0.45
1:KX:283:ARG:HD3	1:LX:94:HIS:NE2	2.31	0.45
1:QX:57:ILE:HG21	1:QX:97:ILE:HD11	1.98	0.45
1:QX:103:LYS:NZ	1:QX:268:GLU:HB3	2.31	0.45
1:EX:276:TRP:O	1:EX:278:THR:HG22	2.17	0.45
1:EX:278:THR:OG1	1:EX:279:ASN:N	2.48	0.45
1:KX:58:TRP:H	1:KX:305:TYR:HD2	1.63	0.45
1:QX:62:ASP:N	1:QX:62:ASP:OD1	2.50	0.45
2:FY:1543:LEU:HD12	2:GY:1526:LEU:HD11	1.99	0.45
2:PY:1510:LEU:HD23	2:PY:1510:LEU:HA	1.76	0.45
1:AX:288:LEU:HD22	1:BX:68:GLN:HE21	1.82	0.45
1:CX:130:LYS:HA	1:DX:120:ARG:HH22	1.81	0.45
1:EX:280:LEU:N	1:EX:291:PHE:O	2.45	0.45
1:IX:93:ASN:ND2	2:HY:1566:ILE:HD13	2.31	0.45
2:LY:1534:ASN:OD1	2:LY:1538:LYS:NZ	2.34	0.45
1:BX:305:TYR:HB3	1:BX:308:VAL:HG13	1.99	0.45
1:DX:58:TRP:H	1:DX:305:TYR:HD2	1.62	0.45
1:GX:66:VAL:HA	1:GX:95:ILE:O	2.17	0.45
1:NX:271:PRO:HA	1:NX:276:TRP:CZ3	2.52	0.45
1:QX:58:TRP:CZ2	2:QY:1476:HIS:HE1	2.35	0.45
1:QX:59:THR:OG1	1:QX:60:SER:N	2.50	0.45
2:DY:1576:ILE:HG21	2:EY:1584:TYR:CE1	2.42	0.45
1:FX:277:ARG:HD2	1:FX:294:ARG:NH1	2.25	0.45
1:JX:80:THR:HG22	1:JX:280:LEU:HD13	1.99	0.45
1:KX:80:THR:HG23	1:KX:280:LEU:HD13	1.99	0.45
1:MX:66:VAL:HG13	1:MX:307:THR:HA	1.99	0.45
1:NX:105:ASN:OD1	1:NX:266:SER:OG	2.21	0.45
1:QX:284:THR:OG1	1:QX:285:ASN:N	2.50	0.45
2:NY:1514:ARG:O	2:NY:1518:GLU:HG2	2.16	0.45
1:EX:57:ILE:HG21	1:EX:97:ILE:HD11	1.99	0.45
1:IX:121:ASP:O	1:IX:124:GLU:HG3	2.17	0.45
1:NX:88:ILE:HG23	1:NX:97:ILE:HG22	1.98	0.45
1:NX:299:ASP:HB2	2:NY:1512:ILE:HD13	1.98	0.45
1:PX:109:GLU:HG3	2:OY:1543:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PX:277:ARG:HH11	1:PX:294:ARG:NH1	2.15	0.45
2:NY:1489:THR:O	2:NY:1491:GLN:NE2	2.47	0.45
1:AX:68:GLN:HE22	1:AX:94:HIS:CD2	2.35	0.44
1:GX:68:GLN:HB3	1:GX:309:LYS:HA	1.99	0.44
1:GX:73:GLU:HG2	1:GX:286:LYS:HB2	1.98	0.44
1:KX:280:LEU:N	1:KX:291:PHE:O	2.36	0.44
1:MX:57:ILE:HG21	1:MX:97:ILE:HD11	1.98	0.44
2:AY:1576:ILE:HG21	2:BY:1584:TYR:CE1	2.52	0.44
2:EY:1487:ASP:OD2	2:EY:1489:THR:OG1	2.32	0.44
1:DX:105:ASN:OD1	1:DX:266:SER:OG	2.27	0.44
1:EX:57:ILE:HD12	1:EX:308:VAL:HG21	2.00	0.44
1:JX:121:ASP:HA	1:JX:124:GLU:HG3	1.98	0.44
1:LX:103:LYS:NZ	1:LX:268:GLU:HB3	2.32	0.44
1:NX:121:ASP:O	1:NX:124:GLU:HG3	2.17	0.44
1:CX:106:LEU:HD21	1:CX:267:ILE:HD13	1.99	0.44
1:CX:305:TYR:HB3	1:CX:308:VAL:HG13	2.00	0.44
1:DX:68:GLN:HA	1:DX:94:HIS:HB3	1.98	0.44
1:DX:103:LYS:NZ	1:DX:268:GLU:HB3	2.31	0.44
1:DX:314:GLN:O	1:DX:317:GLU:HG3	2.18	0.44
1:FX:92:SER:O	1:FX:93:ASN:ND2	2.51	0.44
1:IX:36:ARG:NH1	2:HY:1485:LEU:O	2.33	0.44
2:AY:1526:LEU:HD11	2:QY:1543:LEU:HD12	2.00	0.44
2:CY:1489:THR:O	2:CY:1491:GLN:NE2	2.49	0.44
2:LY:1593:LYS:HD2	2:MY:1603:LEU:HD23	1.99	0.44
1:KX:77:TYR:HB2	1:KX:283:ARG:HH21	1.81	0.44
1:LX:67:ILE:HD11	1:LX:97:ILE:HD13	1.99	0.44
1:PX:59:THR:HG21	1:PX:86:TRP:CZ3	2.53	0.44
1:PX:62:ASP:OD1	1:PX:62:ASP:N	2.50	0.44
2:AY:1586:THR:HG22	2:BY:1599:LEU:HB2	1.97	0.44
2:HY:1509:ILE:HD13	2:HY:1509:ILE:HA	1.80	0.44
2:JY:1576:ILE:HG21	2:KY:1584:TYR:CE1	2.47	0.44
1:BX:59:THR:HG21	1:BX:86:TRP:CZ3	2.52	0.44
1:GX:68:GLN:HA	1:GX:94:HIS:HB3	1.99	0.44
1:GX:305:TYR:HB3	1:GX:308:VAL:HG13	1.99	0.44
1:KX:121:ASP:O	1:KX:124:GLU:HG3	2.18	0.44
1:LX:284:THR:HG23	1:LX:286:LYS:H	1.83	0.44
1:NX:71:LYS:HD3	2:MY:1568:SER:HA	1.99	0.44
1:EX:299:ASP:OD1	1:EX:299:ASP:N	2.37	0.44
1:GX:280:LEU:N	1:GX:291:PHE:O	2.36	0.44
1:OX:61:LEU:HD12	2:NY:1527:ARG:HD3	1.98	0.44
1:OX:283:ARG:HD3	1:PX:94:HIS:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EY:1576:ILE:HG21	2:FY:1584:TYR:CE1	2.46	0.44
2:IY:1475:LEU:HD23	2:IY:1475:LEU:HA	1.84	0.44
2:OY:1536:ALA:HB3	2:PY:1519:VAL:HG23	1.99	0.44
1:FX:68:GLN:HB3	1:FX:309:LYS:HA	2.00	0.44
1:FX:305:TYR:HB3	1:FX:308:VAL:HG13	2.00	0.44
1:GX:126:LEU:HD23	1:GX:126:LEU:HA	1.85	0.44
1:OX:59:THR:HG21	1:OX:86:TRP:CZ3	2.52	0.44
1:EX:70:GLU:OE1	1:EX:315:ARG:NH1	2.49	0.44
1:FX:126:LEU:HD23	1:FX:126:LEU:HA	1.77	0.44
1:IX:59:THR:HG21	1:IX:86:TRP:CZ3	2.53	0.44
1:JX:62:ASP:OD1	1:JX:62:ASP:N	2.51	0.44
1:JX:286:LYS:O	1:JX:315:ARG:NH2	2.50	0.44
2:DY:1535:MET:HE2	2:DY:1544:PRO:HD3	2.00	0.44
1:KX:46:ILE:HG21	1:KX:55:ILE:HG21	1.99	0.44
1:KX:277:ARG:HD2	1:KX:294:ARG:NH1	2.30	0.44
1:NX:102:VAL:HG12	1:NX:103:LYS:N	2.33	0.44
1:OX:308:VAL:O	1:OX:308:VAL:HG13	2.18	0.44
2:FY:1486:ASP:OD1	2:FY:1487:ASP:N	2.50	0.44
2:FY:1586:THR:HG22	2:FY:1590:ILE:HD11	1.99	0.44
2:MY:1514:ARG:O	2:MY:1518:GLU:HG2	2.18	0.44
1:AX:82:PHE:CD1	2:QY:1548:LYS:HD3	2.52	0.43
1:BX:130:LYS:HA	1:CX:120:ARG:HH22	1.83	0.43
1:JX:59:THR:HG21	1:JX:86:TRP:CZ3	2.52	0.43
1:JX:276:TRP:O	1:JX:278:THR:HG22	2.18	0.43
1:NX:62:ASP:OD2	1:NX:62:ASP:N	2.50	0.43
1:NX:103:LYS:NZ	1:NX:268:GLU:HB3	2.33	0.43
1:PX:58:TRP:H	1:PX:305:TYR:HD2	1.66	0.43
2:OY:1485:LEU:HD23	2:OY:1485:LEU:HA	1.88	0.43
2:QY:1487:ASP:OD1	2:QY:1489:THR:OG1	2.35	0.43
1:CX:288:LEU:HD21	1:DX:66:VAL:HG11	2.00	0.43
1:DX:77:TYR:HB2	1:DX:283:ARG:HH21	1.82	0.43
1:DX:284:THR:OG1	1:DX:285:ASN:N	2.49	0.43
1:MX:59:THR:HG21	1:MX:86:TRP:HZ3	1.82	0.43
2:EY:1486:ASP:OD2	2:EY:1487:ASP:N	2.51	0.43
1:CX:78:ILE:HD12	1:CX:95:ILE:HD13	1.99	0.43
1:EX:103:LYS:NZ	1:EX:268:GLU:HB3	2.32	0.43
1:GX:67:ILE:HG23	1:GX:308:VAL:HG23	2.01	0.43
1:JX:310:LEU:HD23	1:JX:310:LEU:HA	1.81	0.43
1:LX:106:LEU:HD21	1:LX:267:ILE:HD13	2.01	0.43
2:AY:1514:ARG:O	2:AY:1518:GLU:HG2	2.17	0.43
2:CY:1502:SER:N	2:CY:1505:GLU:OE1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FY:1514:ARG:O	2:FY:1518:GLU:HG2	2.18	0.43
1:KX:73:GLU:O	1:KX:93:ASN:HA	2.18	0.43
1:QX:106:LEU:HD21	1:QX:267:ILE:HD13	2.01	0.43
1:QX:277:ARG:HD2	1:QX:294:ARG:NH1	2.32	0.43
1:BX:276:TRP:O	1:BX:278:THR:HG22	2.18	0.43
2:AY:1586:THR:HG22	2:BY:1599:LEU:HD22	2.00	0.43
1:EX:68:GLN:HG2	1:EX:309:LYS:HG3	2.00	0.43
1:HX:93:ASN:ND2	2:GY:1566:ILE:HD13	2.34	0.43
1:IX:92:SER:O	1:IX:93:ASN:ND2	2.51	0.43
2:CY:1470:SER:OG	2:CY:1471:LYS:N	2.52	0.43
2:IY:1593:LYS:HB2	2:IY:1593:LYS:HE3	1.67	0.43
1:CX:59:THR:HG21	1:CX:86:TRP:CZ3	2.53	0.43
1:FX:102:VAL:HG12	1:FX:103:LYS:N	2.34	0.43
1:NX:37:GLY:HA2	1:NX:298:LYS:HB2	2.01	0.43
1:PX:279:ASN:HA	1:PX:292:ILE:HA	2.01	0.43
2:KY:1514:ARG:O	2:KY:1518:GLU:HG2	2.18	0.43
1:IX:284:THR:HG23	1:IX:286:LYS:H	1.83	0.43
1:JX:271:PRO:HA	1:JX:276:TRP:CH2	2.54	0.43
1:JX:281:VAL:HG12	1:JX:290:GLN:HE22	1.84	0.43
1:KX:126:LEU:HD23	1:KX:126:LEU:HA	1.84	0.43
1:DX:101:SER:OG	2:BY:1549:ASN:ND2	2.52	0.43
1:EX:101:SER:HA	1:EX:271:PRO:HD3	2.01	0.43
1:GX:36:ARG:NH1	2:FY:1485:LEU:O	2.39	0.43
1:JX:82:PHE:CD1	2:IY:1548:LYS:HD3	2.54	0.43
1:KX:73:GLU:HG2	1:KX:286:LYS:HB2	2.00	0.43
1:MX:314:GLN:O	1:MX:317:GLU:HG3	2.19	0.43
2:CY:1486:ASP:OD1	2:CY:1487:ASP:N	2.52	0.43
2:CY:1579:ASP:OD1	2:CY:1580:ILE:N	2.52	0.43
2:DY:1495:GLU:OE2	2:DY:1506:ARG:NH2	2.52	0.43
1:AX:33:ASN:OD1	1:AX:34:PHE:N	2.52	0.43
1:AX:57:ILE:HD12	1:AX:308:VAL:HG21	2.01	0.43
1:QX:67:ILE:HD11	1:QX:97:ILE:HD13	2.00	0.43
2:EY:1501:LEU:HD22	2:EY:1505:GLU:HB3	2.00	0.43
2:JY:1543:LEU:HD12	2:KY:1526:LEU:HD11	2.01	0.43
1:HX:58:TRP:H	1:HX:305:TYR:HD2	1.64	0.42
1:HX:283:ARG:HD3	1:IX:94:HIS:NE2	2.34	0.42
1:IX:314:GLN:O	1:IX:317:GLU:HG3	2.19	0.42
1:NX:283:ARG:NE	1:OX:94:HIS:CE1	2.87	0.42
1:PX:58:TRP:HH2	1:PX:294:ARG:HH21	1.67	0.42
2:DY:1482:LEU:HD23	2:DY:1482:LEU:HA	1.91	0.42
2:IY:1502:SER:O	2:IY:1506:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DX:73:GLU:O	1:DX:93:ASN:HA	2.19	0.42
1:EX:92:SER:HB3	2:DY:1560:ASN:HA	2.01	0.42
1:IX:73:GLU:O	1:IX:93:ASN:HA	2.19	0.42
1:JX:45:LYS:HD3	1:JX:309:LYS:HB3	2.00	0.42
1:JX:103:LYS:NZ	1:JX:268:GLU:HB3	2.33	0.42
2:BY:1568:SER:OG	2:BY:1569:ASP:N	2.51	0.42
2:JY:1568:SER:OG	2:JY:1569:ASP:N	2.51	0.42
2:OY:1543:LEU:HD12	2:PY:1526:LEU:HD11	2.01	0.42
1:DX:305:TYR:HB3	1:DX:308:VAL:HG13	2.00	0.42
1:HX:305:TYR:HB3	1:HX:308:VAL:HG13	2.00	0.42
1:IX:284:THR:OG1	1:IX:285:ASN:N	2.53	0.42
1:MX:271:PRO:HA	1:MX:276:TRP:CZ3	2.53	0.42
2:LY:1593:LYS:HE2	2:MY:1603:LEU:HA	2.02	0.42
1:AX:284:THR:HG23	1:AX:286:LYS:H	1.84	0.42
1:IX:73:GLU:HG2	1:IX:286:LYS:HB2	2.00	0.42
1:LX:271:PRO:HA	1:LX:276:TRP:CZ3	2.55	0.42
1:MX:277:ARG:HD2	1:MX:294:ARG:NH1	2.33	0.42
1:MX:277:ARG:HE	1:MX:292:ILE:HD11	1.84	0.42
1:OX:277:ARG:HD2	1:OX:294:ARG:NH1	2.28	0.42
1:QX:314:GLN:O	1:QX:317:GLU:HG3	2.20	0.42
2:CY:1530:LYS:HD3	2:CY:1530:LYS:HA	1.88	0.42
1:BX:92:SER:HB2	2:AY:1560:ASN:HA	2.02	0.42
1:DX:271:PRO:HA	1:DX:276:TRP:CZ3	2.55	0.42
1:FX:277:ARG:HH11	1:FX:294:ARG:NH1	2.18	0.42
1:HX:272:SER:HB2	1:HX:297:GLN:HE22	1.85	0.42
1:MX:57:ILE:HD13	1:MX:57:ILE:HA	1.89	0.42
1:MX:121:ASP:O	1:MX:124:GLU:HG3	2.19	0.42
1:MX:297:GLN:H	1:MX:300:ASN:HB2	1.85	0.42
1:PX:314:GLN:O	1:PX:317:GLU:HG3	2.19	0.42
2:KY:1486:ASP:OD1	2:KY:1487:ASP:N	2.52	0.42
2:PY:1482:LEU:HD23	2:PY:1482:LEU:HA	1.90	0.42
2:QY:1475:LEU:HD23	2:QY:1475:LEU:HA	1.87	0.42
1:EX:277:ARG:HD2	1:EX:294:ARG:NH1	2.31	0.42
1:HX:265:ASN:OD1	1:HX:265:ASN:N	2.49	0.42
1:OX:299:ASP:OD1	1:OX:299:ASP:N	2.37	0.42
2:EY:1502:SER:O	2:EY:1506:ARG:HG3	2.20	0.42
2:MY:1509:ILE:HD13	2:MY:1509:ILE:HA	1.86	0.42
2:OY:1486:ASP:OD2	2:OY:1487:ASP:N	2.52	0.42
2:PY:1495:GLU:OE2	2:PY:1506:ARG:NH2	2.52	0.42
1:AX:308:VAL:HG23	1:AX:308:VAL:O	2.19	0.42
1:GX:121:ASP:O	1:GX:124:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PX:305:TYR:HB3	1:PX:308:VAL:HG23	2.02	0.42
2:EY:1586:THR:HG22	2:EY:1590:ILE:HD11	2.01	0.42
1:IX:277:ARG:HD2	1:IX:294:ARG:NH1	2.35	0.42
1:JX:58:TRP:HH2	1:JX:294:ARG:HH21	1.68	0.42
1:LX:70:GLU:OE1	1:LX:315:ARG:NH1	2.51	0.42
1:MX:276:TRP:O	1:MX:278:THR:HG22	2.20	0.42
1:NX:284:THR:HG23	1:NX:287:ALA:H	1.84	0.42
2:GY:1495:GLU:OE2	2:GY:1506:ARG:NH2	2.53	0.42
2:IY:1579:ASP:OD1	2:IY:1580:ILE:N	2.53	0.42
2:NY:1599:LEU:O	2:NY:1603:LEU:HG	2.19	0.42
2:QY:1486:ASP:OD1	2:QY:1487:ASP:N	2.53	0.42
1:BX:102:VAL:HG12	1:BX:103:LYS:N	2.35	0.42
1:LX:62:ASP:OD2	1:LX:62:ASP:N	2.53	0.42
2:GY:1509:ILE:HD13	2:GY:1509:ILE:HA	1.82	0.42
2:IY:1514:ARG:O	2:IY:1518:GLU:HG2	2.20	0.42
2:JY:1586:THR:HG22	2:JY:1590:ILE:HD11	2.02	0.42
2:JY:1599:LEU:O	2:JY:1603:LEU:HG	2.20	0.42
1:AX:284:THR:HG23	1:AX:287:ALA:H	1.85	0.42
1:FX:92:SER:HB2	2:EY:1560:ASN:HA	2.00	0.42
1:IX:77:TYR:CD2	1:JX:96:PHE:HE2	2.38	0.42
1:JX:272:SER:OG	1:JX:297:GLN:NE2	2.50	0.42
1:MX:62:ASP:OD2	2:KY:1548:LYS:NZ	2.53	0.42
1:NX:92:SER:HB3	2:MY:1560:ASN:HA	2.02	0.42
1:NX:278:THR:OG1	1:NX:279:ASN:N	2.52	0.42
2:CY:1535:MET:HE2	2:CY:1544:PRO:HD3	2.02	0.42
2:HY:1514:ARG:O	2:HY:1518:GLU:HG2	2.20	0.42
2:JY:1514:ARG:O	2:JY:1518:GLU:HG2	2.20	0.42
2:QY:1586:THR:HG22	2:QY:1590:ILE:HD11	2.01	0.42
1:AX:70:GLU:OE1	1:AX:315:ARG:NH1	2.53	0.41
1:BX:73:GLU:HG2	1:BX:286:LYS:HB2	2.02	0.41
1:CX:288:LEU:HD22	1:DX:68:GLN:NE2	2.35	0.41
1:EX:121:ASP:O	1:EX:124:GLU:HG3	2.20	0.41
1:HX:77:TYR:HB2	1:HX:283:ARG:HH21	1.85	0.41
1:KX:88:ILE:HG12	1:KX:97:ILE:HG22	2.01	0.41
1:LX:280:LEU:N	1:LX:291:PHE:O	2.39	0.41
1:MX:46:ILE:HG13	1:MX:308:VAL:HG23	2.01	0.41
2:AY:1603:LEU:HA	2:QY:1593:LYS:HE2	2.01	0.41
2:BY:1586:THR:HG22	2:BY:1590:ILE:HD11	2.02	0.41
2:FY:1482:LEU:HD23	2:FY:1482:LEU:HA	1.90	0.41
2:MY:1586:THR:HG22	2:MY:1590:ILE:HD11	2.02	0.41
1:EX:88:ILE:HG22	1:EX:90:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EX:273:ASP:H	1:EX:297:GLN:NE2	2.18	0.41
1:IX:285:ASN:N	1:IX:285:ASN:OD1	2.53	0.41
1:OX:66:VAL:HG13	1:OX:307:THR:HA	2.02	0.41
1:PX:89:VAL:HG13	1:PX:96:PHE:HB2	2.01	0.41
2:HY:1498:LEU:HD23	2:HY:1498:LEU:HA	1.89	0.41
2:JY:1593:LYS:HD2	2:KY:1603:LEU:HD23	2.02	0.41
2:MY:1502:SER:O	2:MY:1506:ARG:HG3	2.20	0.41
1:HX:103:LYS:NZ	1:HX:268:GLU:HB3	2.35	0.41
1:NX:61:LEU:HD21	1:NX:295:ILE:HD13	2.02	0.41
1:NX:310:LEU:HD23	1:NX:310:LEU:HA	1.77	0.41
2:BY:1486:ASP:OD2	2:BY:1487:ASP:N	2.53	0.41
1:GX:273:ASP:H	1:GX:297:GLN:NE2	2.18	0.41
1:JX:88:ILE:HG12	1:JX:97:ILE:HG22	2.01	0.41
1:KX:36:ARG:NH1	2:JY:1485:LEU:O	2.44	0.41
2:FY:1599:LEU:O	2:FY:1603:LEU:HG	2.20	0.41
2:JY:1510:LEU:HD23	2:JY:1510:LEU:HA	1.84	0.41
1:AX:57:ILE:HG21	1:AX:97:ILE:HD11	2.03	0.41
1:FX:301:PHE:O	2:FY:1476:HIS:HB2	2.21	0.41
1:PX:276:TRP:O	1:PX:278:THR:HG22	2.20	0.41
1:PX:284:THR:OG1	1:PX:285:ASN:N	2.53	0.41
2:DY:1510:LEU:HD23	2:DY:1510:LEU:HA	1.79	0.41
2:KY:1587:GLU:HA	2:KY:1590:ILE:HD12	2.02	0.41
1:CX:66:VAL:HG13	1:CX:307:THR:HA	2.02	0.41
1:CX:284:THR:OG1	1:CX:285:ASN:N	2.52	0.41
1:DX:58:TRP:HH2	1:DX:294:ARG:HH21	1.69	0.41
1:HX:283:ARG:HH11	2:HY:1566:ILE:HG12	1.85	0.41
1:HX:314:GLN:O	1:HX:317:GLU:HG3	2.21	0.41
1:JX:73:GLU:O	1:JX:93:ASN:HA	2.20	0.41
1:KX:87:SER:O	2:IY:1553:ILE:HD11	2.20	0.41
1:LX:284:THR:OG1	1:LX:285:ASN:N	2.53	0.41
1:LX:314:GLN:O	1:LX:317:GLU:HG3	2.21	0.41
2:FY:1576:ILE:HG21	2:GY:1584:TYR:CE1	2.56	0.41
2:IY:1498:LEU:HD11	2:IY:1510:LEU:HD21	2.03	0.41
1:AX:73:GLU:O	1:AX:93:ASN:HA	2.21	0.41
1:AX:277:ARG:HD2	1:AX:294:ARG:NH1	2.31	0.41
1:DX:283:ARG:HB2	1:DX:288:LEU:HD12	2.03	0.41
1:DX:310:LEU:HD23	1:DX:310:LEU:HA	1.91	0.41
1:HX:310:LEU:HD23	1:HX:310:LEU:HA	1.82	0.41
1:IX:271:PRO:HA	1:IX:276:TRP:CZ3	2.56	0.41
1:OX:280:LEU:N	1:OX:291:PHE:O	2.39	0.41
2:DY:1486:ASP:OD2	2:DY:1487:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IY:1562:ASP:N	2:IY:1562:ASP:OD1	2.54	0.41
2:IY:1586:THR:HG22	2:IY:1590:ILE:HD11	2.03	0.41
1:CX:57:ILE:HD13	1:CX:57:ILE:HA	1.93	0.41
1:CX:92:SER:HB3	2:BY:1561:VAL:HG12	2.03	0.41
1:FX:310:LEU:HA	1:FX:310:LEU:HD23	1.79	0.41
1:GX:314:GLN:O	1:GX:317:GLU:HG3	2.21	0.41
1:MX:48:TYR:HB2	1:MX:310:LEU:HD22	2.01	0.41
1:NX:102:VAL:HG23	1:NX:276:TRP:HZ2	1.86	0.41
2:CY:1475:LEU:HD21	2:CY:1505:GLU:HB3	2.02	0.41
2:DY:1548:LYS:HG3	2:EY:1527:ARG:HH22	1.86	0.41
2:HY:1586:THR:HG22	2:HY:1590:ILE:HD11	2.01	0.41
2:LY:1599:LEU:O	2:LY:1603:LEU:HG	2.21	0.41
2:QY:1530:LYS:HD3	2:QY:1530:LYS:HA	1.90	0.41
1:BX:301:PHE:O	2:BY:1476:HIS:HB2	2.21	0.41
1:DX:73:GLU:CD	1:DX:289:TYR:HH	2.23	0.41
1:JX:102:VAL:HG12	1:JX:103:LYS:N	2.36	0.41
2:AY:1530:LYS:HD3	2:AY:1530:LYS:HA	1.94	0.41
2:AY:1543:LEU:HD12	2:BY:1526:LEU:HD11	2.02	0.41
2:FY:1586:THR:HG23	2:GY:1599:LEU:HB2	2.03	0.41
2:HY:1502:SER:O	2:HY:1506:ARG:HG3	2.20	0.41
2:JY:1530:LYS:HD3	2:JY:1530:LYS:HA	1.83	0.41
2:MY:1593:LYS:HB2	2:MY:1593:LYS:HE3	1.74	0.41
2:OY:1579:ASP:OD1	2:OY:1580:ILE:N	2.54	0.41
1:CX:73:GLU:O	1:CX:93:ASN:HA	2.21	0.41
1:DX:276:TRP:O	1:DX:278:THR:HG22	2.21	0.41
1:IX:62:ASP:OD1	1:IX:62:ASP:N	2.54	0.41
1:JX:271:PRO:HA	1:JX:276:TRP:CE3	2.56	0.41
1:JX:278:THR:OG1	1:JX:279:ASN:N	2.54	0.41
1:PX:56:THR:HA	1:PX:292:ILE:HG23	2.03	0.41
1:PX:271:PRO:HA	1:PX:276:TRP:CZ3	2.56	0.41
2:CY:1536:ALA:HB3	2:DY:1519:VAL:HG23	2.03	0.41
2:EY:1523:TYR:OH	2:EY:1527:ARG:NH2	2.35	0.41
2:GY:1514:ARG:O	2:GY:1518:GLU:HG2	2.20	0.41
2:IY:1530:LYS:HD3	2:IY:1530:LYS:HA	1.92	0.41
2:LY:1482:LEU:HD13	2:LY:1513:LYS:HD2	2.03	0.41
2:LY:1586:THR:HG22	2:LY:1590:ILE:HD11	2.03	0.41
2:OY:1495:GLU:OE2	2:OY:1506:ARG:NH2	2.54	0.41
1:AX:88:ILE:HG12	1:AX:97:ILE:HG22	2.04	0.40
1:KX:288:LEU:HD22	1:LX:68:GLN:NE2	2.36	0.40
1:NX:57:ILE:HD12	1:NX:308:VAL:HG21	2.03	0.40
1:OX:59:THR:HG21	1:OX:86:TRP:CH2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:PX:299:ASP:HB2	2:PY:1512:ILE:HD13	2.03	0.40
2:BY:1579:ASP:HB3	2:BY:1582:LYS:HD3	2.03	0.40
2:DY:1530:LYS:HD3	2:DY:1530:LYS:HA	1.91	0.40
2:IY:1489:THR:O	2:IY:1491:GLN:NE2	2.49	0.40
1:CX:70:GLU:OE1	1:CX:315:ARG:NH1	2.54	0.40
1:EX:58:TRP:CZ2	2:EY:1476:HIS:HE1	2.39	0.40
1:GX:61:LEU:HD12	2:FY:1527:ARG:HD3	2.03	0.40
1:LX:73:GLU:O	1:LX:93:ASN:HA	2.22	0.40
1:LX:276:TRP:O	1:LX:278:THR:HG22	2.21	0.40
1:NX:306:LEU:HD23	1:NX:306:LEU:HA	1.86	0.40
1:OX:280:LEU:HB2	1:OX:293:LEU:HD11	2.03	0.40
2:AY:1576:ILE:HG21	2:BY:1584:TYR:HE1	1.84	0.40
2:AY:1584:TYR:CE1	2:QY:1576:ILE:HG21	2.45	0.40
2:QY:1510:LEU:HD23	2:QY:1510:LEU:HA	1.82	0.40
1:AX:306:LEU:HD22	1:QX:279:ASN:ND2	2.37	0.40
1:AX:317:GLU:O	1:AX:321:VAL:HG13	2.22	0.40
1:BX:77:TYR:HA	2:AY:1555:THR:HG23	2.03	0.40
1:BX:102:VAL:HG23	1:BX:276:TRP:HZ2	1.86	0.40
1:FX:68:GLN:HE22	1:FX:94:HIS:CD2	2.40	0.40
1:FX:93:ASN:ND2	2:EY:1566:ILE:HD13	2.37	0.40
1:GX:58:TRP:H	1:GX:305:TYR:HD2	1.68	0.40
1:KX:53:LYS:HD2	1:KX:53:LYS:HA	1.94	0.40
1:MX:57:ILE:HD12	1:MX:308:VAL:HG11	2.03	0.40
1:NX:71:LYS:HE2	2:MY:1566:ILE:HB	2.02	0.40
1:OX:66:VAL:HA	1:OX:95:ILE:O	2.22	0.40
1:OX:312:TYR:HB3	1:OX:315:ARG:HB2	2.04	0.40
1:AX:102:VAL:HG23	1:AX:276:TRP:HZ2	1.85	0.40
1:FX:265:ASN:OD1	1:FX:265:ASN:N	2.53	0.40
1:IX:106:LEU:HD21	1:IX:267:ILE:HD13	2.03	0.40
1:MX:68:GLN:HB3	1:MX:309:LYS:HA	2.04	0.40
1:QX:68:GLN:HA	1:QX:94:HIS:HB3	2.02	0.40
2:AY:1502:SER:O	2:AY:1506:ARG:HG3	2.22	0.40
1:HX:271:PRO:HA	1:HX:276:TRP:CZ3	2.56	0.40
1:IX:107:MET:N	2:HY:1543:LEU:O	2.51	0.40
1:JX:73:GLU:HG2	1:JX:286:LYS:HB2	2.03	0.40
1:NX:284:THR:OG1	1:NX:285:ASN:N	2.54	0.40
1:PX:310:LEU:HD23	1:PX:310:LEU:HA	1.82	0.40
2:AY:1509:ILE:HD13	2:AY:1509:ILE:HA	1.92	0.40
2:CY:1593:LYS:HD2	2:DY:1603:LEU:HD23	2.03	0.40
2:NY:1482:LEU:HD23	2:NY:1482:LEU:HA	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	BX	160/521 (31%)	151 (94%)	9 (6%)	0	100	100
1	CX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	DX	160/521 (31%)	156 (98%)	4 (2%)	0	100	100
1	EX	160/521 (31%)	153 (96%)	7 (4%)	0	100	100
1	FX	160/521 (31%)	152 (95%)	8 (5%)	0	100	100
1	GX	160/521 (31%)	153 (96%)	7 (4%)	0	100	100
1	HX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	IX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	JX	160/521 (31%)	151 (94%)	9 (6%)	0	100	100
1	KX	160/521 (31%)	157 (98%)	3 (2%)	0	100	100
1	LX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	MX	160/521 (31%)	155 (97%)	5 (3%)	0	100	100
1	NX	160/521 (31%)	156 (98%)	4 (2%)	0	100	100
1	OX	160/521 (31%)	152 (95%)	8 (5%)	0	100	100
1	PX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
1	QX	160/521 (31%)	154 (96%)	6 (4%)	0	100	100
2	AY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	BY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	CY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
2	DY	133/1927 (7%)	126 (95%)	7 (5%)	0	100	100
2	EY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	FY	133/1927 (7%)	123 (92%)	10 (8%)	0	100	100
2	GY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
2	HY	133/1927 (7%)	126 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	IY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
2	JY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	KY	133/1927 (7%)	126 (95%)	7 (5%)	0	100	100
2	LY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	MY	133/1927 (7%)	126 (95%)	7 (5%)	0	100	100
2	NY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	OY	133/1927 (7%)	129 (97%)	4 (3%)	0	100	100
2	PY	133/1927 (7%)	127 (96%)	6 (4%)	0	100	100
2	QY	133/1927 (7%)	128 (96%)	5 (4%)	0	100	100
All	All	4981/41616 (12%)	4775 (96%)	206 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AX	152/469 (32%)	143 (94%)	9 (6%)	16	44
1	BX	152/469 (32%)	142 (93%)	10 (7%)	14	41
1	CX	152/469 (32%)	143 (94%)	9 (6%)	16	44
1	DX	152/469 (32%)	145 (95%)	7 (5%)	23	52
1	EX	152/469 (32%)	140 (92%)	12 (8%)	10	34
1	FX	152/469 (32%)	146 (96%)	6 (4%)	27	56
1	GX	152/469 (32%)	142 (93%)	10 (7%)	14	41
1	HX	152/469 (32%)	143 (94%)	9 (6%)	16	44
1	IX	152/469 (32%)	142 (93%)	10 (7%)	14	41
1	JX	152/469 (32%)	143 (94%)	9 (6%)	16	44
1	KX	152/469 (32%)	142 (93%)	10 (7%)	14	41
1	LX	152/469 (32%)	140 (92%)	12 (8%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	MX	152/469 (32%)	143 (94%)	9 (6%)	16	44
1	NX	152/469 (32%)	147 (97%)	5 (3%)	33	61
1	OX	152/469 (32%)	141 (93%)	11 (7%)	12	37
1	PX	152/469 (32%)	146 (96%)	6 (4%)	27	56
1	QX	152/469 (32%)	142 (93%)	10 (7%)	14	41
2	AY	115/1724 (7%)	112 (97%)	3 (3%)	41	66
2	BY	115/1724 (7%)	111 (96%)	4 (4%)	31	59
2	CY	115/1724 (7%)	111 (96%)	4 (4%)	31	59
2	DY	115/1724 (7%)	110 (96%)	5 (4%)	25	54
2	EY	115/1724 (7%)	114 (99%)	1 (1%)	75	86
2	FY	115/1724 (7%)	112 (97%)	3 (3%)	41	66
2	GY	115/1724 (7%)	112 (97%)	3 (3%)	41	66
2	HY	115/1724 (7%)	111 (96%)	4 (4%)	31	59
2	IY	115/1724 (7%)	111 (96%)	4 (4%)	31	59
2	JY	115/1724 (7%)	113 (98%)	2 (2%)	56	75
2	KY	115/1724 (7%)	112 (97%)	3 (3%)	41	66
2	LY	115/1724 (7%)	111 (96%)	4 (4%)	31	59
2	MY	115/1724 (7%)	111 (96%)	4 (4%)	31	59
2	NY	115/1724 (7%)	111 (96%)	4 (4%)	31	59
2	OY	115/1724 (7%)	112 (97%)	3 (3%)	41	66
2	PY	115/1724 (7%)	111 (96%)	4 (4%)	31	59
2	QY	115/1724 (7%)	110 (96%)	5 (4%)	25	54
All	All	4539/37281 (12%)	4325 (95%)	214 (5%)	24	51

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AX	59	THR
1	AX	62	ASP
1	AX	63	ASN
1	AX	104	SER
1	AX	113	VAL
1	AX	118	MET
1	AX	264	ASP

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Mol	Chain	Res	Type
1	AX	270	SER
1	AX	317	GLU
1	BX	41	VAL
1	BX	59	THR
1	BX	63	ASN
1	BX	93	ASN
1	BX	113	VAL
1	BX	114	ASN
1	BX	124	GLU
1	BX	126	LEU
1	BX	264	ASP
1	BX	317	GLU
1	CX	43	ASN
1	CX	63	ASN
1	CX	93	ASN
1	CX	113	VAL
1	CX	114	ASN
1	CX	124	GLU
1	CX	126	LEU
1	CX	267	ILE
1	CX	317	GLU
1	DX	41	VAL
1	DX	63	ASN
1	DX	93	ASN
1	DX	102	VAL
1	DX	113	VAL
1	DX	114	ASN
1	DX	317	GLU
1	EX	59	THR
1	EX	63	ASN
1	EX	93	ASN
1	EX	113	VAL
1	EX	114	ASN
1	EX	121	ASP
1	EX	124	GLU
1	EX	270	SER
1	EX	278	THR
1	EX	299	ASP
1	EX	317	GLU
1	EX	321	VAL
1	FX	41	VAL
1	FX	63	ASN

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Mol	Chain	Res	Type
1	FX	93	ASN
1	FX	104	SER
1	FX	113	VAL
1	FX	284	THR
1	GX	49	LEU
1	GX	59	THR
1	GX	62	ASP
1	GX	63	ASN
1	GX	93	ASN
1	GX	113	VAL
1	GX	124	GLU
1	GX	278	THR
1	GX	284	THR
1	GX	317	GLU
1	HX	49	LEU
1	HX	62	ASP
1	HX	63	ASN
1	HX	80	THR
1	HX	93	ASN
1	HX	113	VAL
1	HX	267	ILE
1	HX	278	THR
1	HX	317	GLU
1	IX	43	ASN
1	IX	62	ASP
1	IX	63	ASN
1	IX	77	TYR
1	IX	93	ASN
1	IX	113	VAL
1	IX	114	ASN
1	IX	124	GLU
1	IX	278	THR
1	IX	317	GLU
1	JX	59	THR
1	JX	62	ASP
1	JX	63	ASN
1	JX	93	ASN
1	JX	104	SER
1	JX	113	VAL
1	JX	114	ASN
1	JX	264	ASP
1	JX	284	THR

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Mol	Chain	Res	Type
1	KX	63	ASN
1	KX	93	ASN
1	KX	113	VAL
1	KX	120	ARG
1	KX	264	ASP
1	KX	270	SER
1	KX	284	THR
1	KX	299	ASP
1	KX	308	VAL
1	KX	317	GLU
1	LX	43	ASN
1	LX	62	ASP
1	LX	63	ASN
1	LX	80	THR
1	LX	93	ASN
1	LX	104	SER
1	LX	113	VAL
1	LX	114	ASN
1	LX	124	GLU
1	LX	267	ILE
1	LX	278	THR
1	LX	317	GLU
1	MX	62	ASP
1	MX	63	ASN
1	MX	78	ILE
1	MX	113	VAL
1	MX	114	ASN
1	MX	124	GLU
1	MX	270	SER
1	MX	278	THR
1	MX	317	GLU
1	NX	59	THR
1	NX	62	ASP
1	NX	80	THR
1	NX	93	ASN
1	NX	113	VAL
1	OX	43	ASN
1	OX	63	ASN
1	OX	82	PHE
1	OX	93	ASN
1	OX	94	HIS
1	OX	113	VAL

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Mol	Chain	Res	Type
1	OX	114	ASN
1	OX	120	ARG
1	OX	264	ASP
1	OX	299	ASP
1	OX	317	GLU
1	PX	62	ASP
1	PX	63	ASN
1	PX	93	ASN
1	PX	113	VAL
1	PX	267	ILE
1	PX	317	GLU
1	QX	62	ASP
1	QX	63	ASN
1	QX	93	ASN
1	QX	102	VAL
1	QX	113	VAL
1	QX	264	ASP
1	QX	267	ILE
1	QX	278	THR
1	QX	308	VAL
1	QX	317	GLU
2	AY	1497	CYS
2	AY	1514	ARG
2	AY	1520	ASP
2	BY	1479	SER
2	BY	1497	CYS
2	BY	1514	ARG
2	BY	1520	ASP
2	CY	1481	CYS
2	CY	1509	ILE
2	CY	1520	ASP
2	CY	1599	LEU
2	DY	1470	SER
2	DY	1479	SER
2	DY	1497	CYS
2	DY	1514	ARG
2	DY	1520	ASP
2	EY	1497	CYS
2	FY	1497	CYS
2	FY	1514	ARG
2	FY	1520	ASP
2	GY	1497	CYS

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Mol	Chain	Res	Type
2	GY	1520	ASP
2	GY	1579	ASP
2	HY	1479	SER
2	HY	1481	CYS
2	HY	1497	CYS
2	HY	1514	ARG
2	IY	1479	SER
2	IY	1497	CYS
2	IY	1514	ARG
2	IY	1520	ASP
2	JY	1481	CYS
2	JY	1499	GLU
2	KY	1497	CYS
2	KY	1514	ARG
2	KY	1520	ASP
2	LY	1497	CYS
2	LY	1509	ILE
2	LY	1514	ARG
2	LY	1520	ASP
2	MY	1497	CYS
2	MY	1514	ARG
2	MY	1520	ASP
2	MY	1577	GLU
2	NY	1497	CYS
2	NY	1499	GLU
2	NY	1514	ARG
2	NY	1594	ASN
2	OY	1479	SER
2	OY	1509	ILE
2	OY	1520	ASP
2	PY	1479	SER
2	PY	1497	CYS
2	PY	1514	ARG
2	PY	1520	ASP
2	QY	1479	SER
2	QY	1497	CYS
2	QY	1520	ASP
2	QY	1555	THR
2	QY	1577	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	AX	43	ASN
1	AX	68	GLN
1	AX	93	ASN
1	BX	93	ASN
1	BX	94	HIS
1	CX	68	GLN
1	CX	290	GLN
1	DX	68	GLN
1	DX	93	ASN
1	DX	94	HIS
1	DX	297	GLN
1	EX	68	GLN
1	EX	297	GLN
1	FX	93	ASN
1	FX	297	GLN
1	GX	68	GLN
1	GX	297	GLN
1	HX	68	GLN
1	HX	93	ASN
1	HX	297	GLN
1	IX	93	ASN
1	IX	94	HIS
1	JX	68	GLN
1	JX	93	ASN
1	JX	94	HIS
1	JX	297	GLN
1	KX	93	ASN
1	LX	68	GLN
1	LX	94	HIS
1	LX	297	GLN
1	MX	68	GLN
1	MX	93	ASN
1	MX	297	GLN
1	NX	63	ASN
1	NX	68	GLN
1	NX	93	ASN
1	OX	68	GLN
1	OX	93	ASN
1	OX	265	ASN
1	PX	68	GLN
1	PX	93	ASN
1	PX	297	GLN
1	QX	68	GLN

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Mol	Chain	Res	Type
1	QX	93	ASN
2	AY	1549	ASN
2	AY	1557	ASN
2	AY	1583	GLN
2	AY	1594	ASN
2	BY	1476	HIS
2	BY	1549	ASN
2	BY	1557	ASN
2	BY	1583	GLN
2	CY	1476	HIS
2	CY	1528	ASN
2	CY	1557	ASN
2	CY	1583	GLN
2	CY	1594	ASN
2	DY	1549	ASN
2	DY	1557	ASN
2	DY	1583	GLN
2	EY	1476	HIS
2	EY	1557	ASN
2	EY	1583	GLN
2	FY	1476	HIS
2	FY	1528	ASN
2	FY	1549	ASN
2	FY	1583	GLN
2	FY	1594	ASN
2	GY	1476	HIS
2	GY	1549	ASN
2	GY	1557	ASN
2	GY	1583	GLN
2	HY	1549	ASN
2	HY	1583	GLN
2	HY	1594	ASN
2	IY	1476	HIS
2	IY	1549	ASN
2	IY	1583	GLN
2	IY	1594	ASN
2	JY	1476	HIS
2	JY	1549	ASN
2	JY	1557	ASN
2	JY	1583	GLN
2	JY	1594	ASN
2	KY	1476	HIS

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Mol	Chain	Res	Type
2	KY	1549	ASN
2	KY	1557	ASN
2	KY	1583	GLN
2	LY	1476	HIS
2	LY	1549	ASN
2	LY	1557	ASN
2	LY	1583	GLN
2	LY	1594	ASN
2	MY	1476	HIS
2	MY	1549	ASN
2	MY	1557	ASN
2	MY	1583	GLN
2	MY	1594	ASN
2	NY	1476	HIS
2	NY	1549	ASN
2	NY	1583	GLN
2	NY	1594	ASN
2	OY	1476	HIS
2	OY	1557	ASN
2	OY	1583	GLN
2	OY	1594	ASN
2	PY	1549	ASN
2	PY	1557	ASN
2	PY	1583	GLN
2	PY	1594	ASN
2	QY	1476	HIS
2	QY	1528	ASN
2	QY	1549	ASN
2	QY	1557	ASN
2	QY	1583	GLN
2	QY	1594	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-20021. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

This section was not generated.

6.2 Central slices ⓘ

This section was not generated.

6.3 Largest variance slices ⓘ

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

This section was not generated.

6.5 Orthogonal surface views ⓘ

This section was not generated.

6.6 Mask visualisation ⓘ

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.