



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:05 am GMT

PDB ID : 1Q5A
EMDB ID: : EMD-1052
Title : S-shaped trans interactions of cadherins model based on fitting C-cadherin (1L3W) to 3D map of desmosomes obtained by electron tomography
Authors : He, W.; Cowin, P.; Stokes, D.L.
Deposited on : 2003-08-06
Resolution : 30.00 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

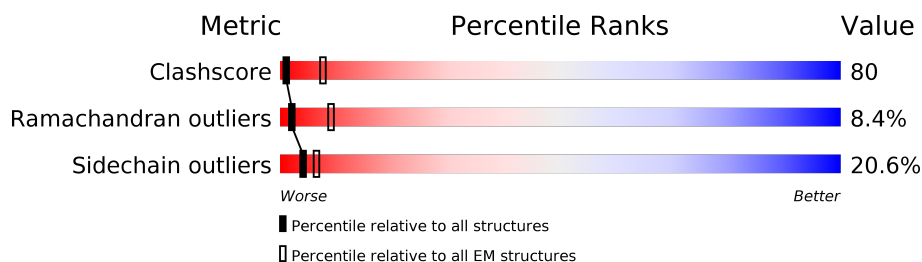
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 30.00 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	880	
1	B	880	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	801	-	-	X	-
2	NAG	A	805	X	-	X	-
2	NAG	A	806	X	-	X	-
2	NAG	A	807	-	-	X	-
2	NAG	A	809	-	-	X	-
2	NAG	A	810	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	904	-	-	X	-
2	NAG	B	801	-	-	X	-
2	NAG	B	805	X	-	X	-
2	NAG	B	806	X	-	X	-
2	NAG	B	807	-	-	X	-
2	NAG	B	809	-	-	X	-
2	NAG	B	810	-	-	X	-
2	NAG	B	904	-	-	X	-
3	NDG	A	902	-	-	X	-
3	NDG	B	811	-	-	X	-
3	NDG	B	902	-	-	X	-

2 Entry composition [i](#)

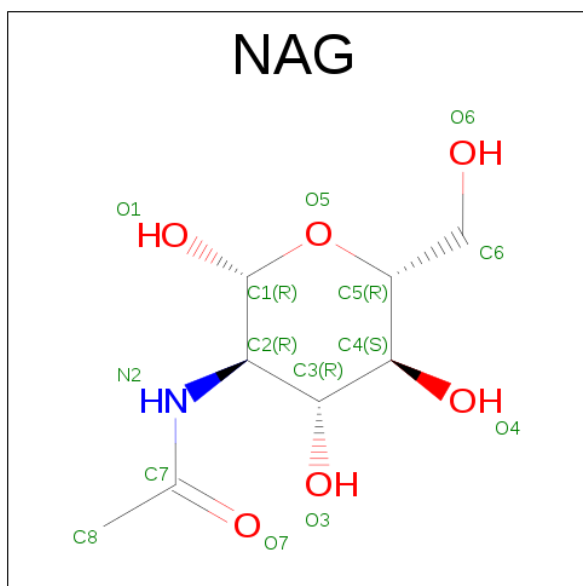
There are 4 unique types of molecules in this entry. The entry contains 8826 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EP-cadherin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		
1	B	540	Total	C	N	O	S	0	0
			4191	2635	695	850	11		

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



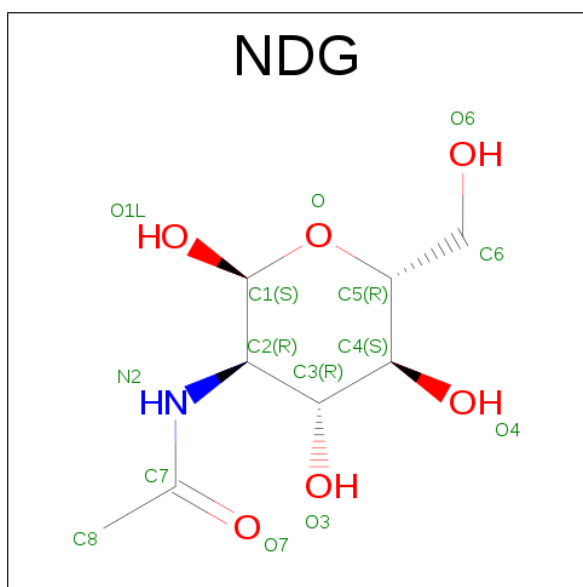
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	

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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	A	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	
2	B	1	Total	C	N	O	0
			154	88	11	55	

- Molecule 3 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	B	1	Total	C	N	O	0
			56	32	4	20	
3	B	1	Total	C	N	O	0
			56	32	4	20	
3	B	1	Total	C	N	O	0
			56	32	4	20	

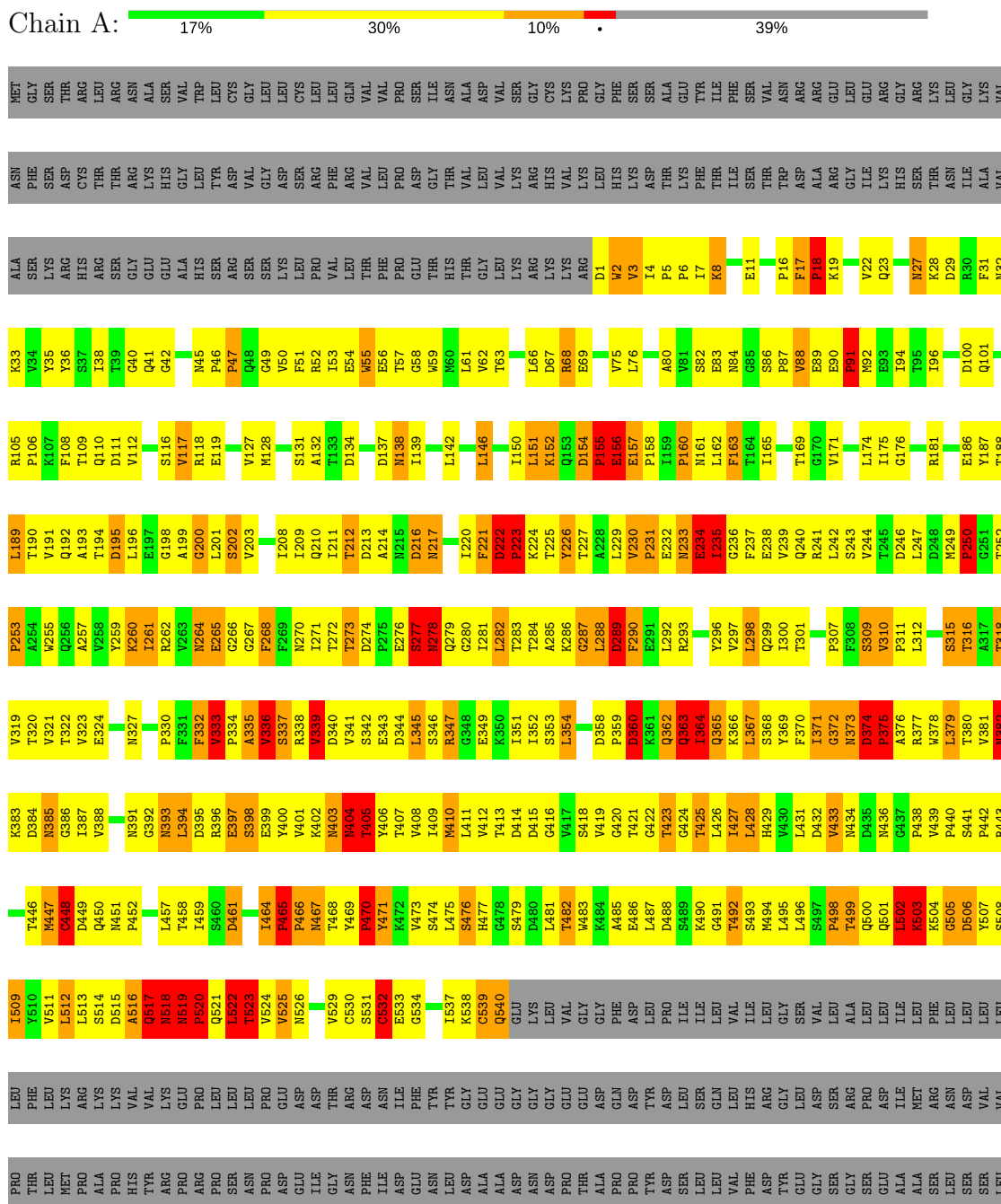
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	B	12	Total	Ca	0
			12	12	
4	A	12	Total	Ca	0
			12	12	

3 Residue-property plots

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



ASN	SER	SER	ASN	SER	ASN	ASP	GLU	HIS	ASP	TYR	ASN	TYR	LEU	SER	ASP	TRP	GLY	SER	ARG	PHE	ARG	LYS	LEU	ALA	ASP	MET	TYR	GLY	GLY	ASP	ASP	ASP	GLU	GLU
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- Molecule 1: EP-cadherin

Chain B: 16% 30% 11% 1% 42%

MET		Gly	SER	THR	ARG	LEU	ASN	ALA	SER	VAL	TRP	LEU	CYS	GLY	LEU	CYS	LEU	GLN	VAL	ASP	PRO	SER	ILE	ASN	ASP	VAL	SER	GLY	Lys	PHE	SER	SER	ALA	GLU	Tyr	ILE	PHE	SER	Val	ASN	Arg	Leu	Glut	Thr	Met
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ASN	PHE	SER	ASP	CYS	THR	THR	ARG	ARG	LYS	HIS	GLY	LEU	TYR	ASP	VAL	GLY	ASP	SER	SER	ARG	PHE	ARG	ARG	ARG	VAL	LEU	PRO	ASP	GLY	THR	GLY	VAL	LEU	VAL	LYS	ARG	HIS	VAL	LYS	LYS	HIS	LEU	LYS	ASP	ASP	THR	THR	PHE	THR	ILE	SER	THR	THR	TRP	ASP	ALA	ALA	ARG	GLY	ILE	LYS	HIS	SER	THR	THR	ASN	ALA	ALA
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ALA	SER	LYS	ARG	HIS	ARG	SER	GLY	GLU	GLU	ALA	HIS	SER	ARG	SER	SER	LYS	LEU	PRO	VAL	LEU	THR	THR	PRO	GLU	GLU	HIS	HIS	THR	GLY	LEU	LYS	LYS	ARG	ARG	D1	W2	W2	V3	I4	I4	P5	P6	I7	I7	K8	K8	E11	P16	F17	P18	K19	V22	Q23	I24	K25	S26	N27	K28	D29
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F31	N32	K33	Y36	S37	I38	T39	G40	Q41	G42	M45	P46	P47	G48	G49	V50	F51	R52	I53	E54	E55	E56	T57	G58	V59	M60	L61	V62	T63	L66	D67	R68	E69	V75	L76	S77	H79	A80	E83	S86	P87	V88	E89	E90	P91	E92	M93	I94	T95	I96	D100
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L105	L106	L107	L108	L109	L110	L111	L112	S116	L117	L118	L119	L120	L121	L122	L123	L124	L125	L126	L127	L128	L129	L130	L131	L132	L133	L134	L135	L136	L137	L138	L139	L140	L141	L142	L143	L144	L145	L146	L147	L148	L149	L150	L151	L152	L153	L154	L155	L156	L157	L158	L159	L160	L161	L162	L163	L164	L165	L166	L167	L168	L169	L170	L171	L172	L173	L174	L175	L176	L177	L178	L179	L180	L181	L182	L183	L184	L185	L186	L187	L188	L189	L190	L191	L192	L193	L194	L195	L196	L197	L198	L199	L200	L201	L202	L203	L204	L205	L206	L207	L208	L209	L210	L211	L212	L213	L214	L215	L216	L217	L218	L219	L220	L221	L222	L223	L224	L225	L226	L227	L228	L229	L230	L231	L232	L233	L234	L235	L236	L237	L238	L239	L240	L241	L242	L243	L244	L245	L246	L247	L248	L249	L250	L251	L252	L253	L254	L255	L256	L257	L258	L259	L260	L261	L262	L263	L264	L265	L266	L267	L268	L269	L270	L271	L272	L273	L274	L275	L276	L277	L278	L279	L280	L281	L282	L283	L284	L285	L286	L287	L288	L289	L290	L291	L292	L293	L294	L295	L296	L297	L298	L299	L300	L301	L302	L303	L304	L305	L306	L307	L308	L309	L310	L311	L312	L313	L314	L315	L316	L317	L318	L319	L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354	L355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618
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R181		E186	IY17	T188	L189	T190	IY191	Q192	A193	T194	D195	L196	E197	G198	A199	L201	S202	V203	Z208	L208	L209	Q210	I211	T212	D213	D216	N217	L220	F221	D222	F223	K224	T225	Y226	T227	A228	L229	Z230	P231	E232	N233	E234	L235	G236	F237	E238	V239	Q240	R241	L242	S243	V244	D245	T246	L247
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Y249	Y250	G251	Y252	Y253	Y254	Y255	Y256	Y257	Y258	Y259	Y260	Y261	Y262	Y263	Y264	Y265	Y266	Y267	Y268	Y269	Y270	Y271	Y272	Y273	Y274	Y275	Y276	Y277	Y278	Y279	Y280	Y281	Y282	Y283	Y284	Y285	Y286	Y287	Y288	Y289	Y290	Y291	Y292	Y293	Y294	Y295	Y296	Y297	Y298	Y299	Y300	Y301	Y302	Y303	Y304	Y305	Y306	Y307	Y308	Y309	Y310	Y311	Y312	Y313	Y314	Y315	Y316	Y317	Y318	Y319	Y320	Y321	Y322	Y323	Y324	Y325	Y326	Y327	Y328	Y329	Y330	Y331	Y332	Y333	Y334	Y335	Y336	Y337	Y338	Y339	Y340	Y341	Y342	Y343	Y344	Y345	Y346	Y347	Y348	Y349	Y350	Y351	Y352	Y353	Y354	Y355	Y356	Y357	Y358	Y359	Y360	Y361	Y362	Y363	Y364	Y365	Y366	Y367	Y368	Y369	Y370	Y371	Y372	Y373	Y374	Y375	Y376	Y377	Y378	Y379	Y380	Y381	Y382	Y383	Y384	Y385	Y386	Y387	Y388	Y389	Y390	Y391	Y392	Y393	Y394	Y395	Y396	Y397	Y398	Y399	Y400	Y401	Y402	Y403	Y404	Y405	Y406	Y407	Y408	Y409	Y410	Y411	Y412	Y413	Y414	Y415	Y416	Y417	Y418	Y419	Y420	Y421	Y422	Y423	Y424	Y425	Y426	Y427	Y428	Y429	Y430	Y431	Y432	Y433	Y434	Y435	Y436	Y437	Y438	Y439	Y440	Y441	Y442	Y443	Y444	Y445	Y446	Y447	Y448	Y449	Y450	Y451	Y452	Y453	Y454	Y455	Y456	Y457	Y458	Y459	Y460	Y461	Y462	Y463	Y464	Y465	Y466	Y467	Y468	Y469	Y470	Y471	Y472	Y473	Y474	Y475	Y476	Y477	Y478	Y479	Y480	Y481	Y482	Y483	Y484	Y485	Y486	Y487	Y488	Y489	Y490	Y491	Y492	Y493	Y494	Y495	Y496	Y497	Y498	Y499	Y500	Y501	Y502	Y503	Y504	Y505	Y506	Y507	Y508	Y509	Y510	Y511	Y512	Y513	Y514	Y515	Y516	Y517	Y518	Y519	Y520	Y521	Y522	Y523	Y524	Y525	Y526	Y527	Y528	Y529	Y530	Y531	Y532	Y533	Y534	Y535	Y536	Y537	Y538	Y539	Y540	Y541	Y542	Y543	Y544	Y545	Y546	Y547	Y548	Y549	Y550	Y551	Y552	Y553	Y554	Y555	Y556	Y557	Y558	Y559	Y560	Y561	Y562	Y563	Y564	Y565	Y566	Y567	Y568	Y569	Y570	Y571	Y572	Y573	Y574	Y575	Y576	Y577	Y578	Y579	Y580	Y581	Y582	Y583	Y584	Y585	Y586	Y587	Y588	Y589	Y590	Y591	Y592	Y593	Y594	Y595	Y596	Y597	Y598	Y599	Y600	Y601	Y602	Y603	Y604	Y605	Y606	Y607	Y608	Y609	Y610	Y611	Y612	Y613	Y614	Y615	Y616	Y617	Y618	Y619	Y620	Y621	Y622	Y623	Y624	Y625	Y626	Y627	Y628	Y629	Y630	Y631	Y632	Y633	Y634	Y635	Y636	Y637	Y638	Y639	Y640	Y641	Y642	Y643	Y644	Y645	Y646	Y647	Y648	Y649	Y650	Y651	Y652	Y653	Y654	Y655	Y656	Y657	Y658	Y659	Y660	Y661	Y662	Y663	Y664	Y665	Y666	Y667	Y668	Y669	Y670	Y671	Y672	Y673	Y674	Y675	Y676	Y677	Y678	Y679	Y680	Y681	Y682	Y683	Y684	Y685	Y686	Y687	Y688	Y689	Y690	Y691	Y692	Y693	Y694	Y695	Y696	Y697	Y698	Y699	Y700	Y701	Y702	
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S315	A316	A317	A318	A319	A320	A321	A322	A323	A324	A325	A326	A327	A328	A329	A330	A331	A332	A333	A334	A335	A336	A337	A338	A339	A340	A341	A342	A343	A344	A345	A346	A347	A348	A349	A350	A351	A352	A353	A354	A355	A356	A357	A358	A359	A360	A361	A362	A363	A364	A365	A366	A367	A368	A369	A370	A371	A372	A373	A374	A375	A376	A377
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L379	T380	V381	N382	K383	D384	G385	H386	I387	V388		N391	G392	N393	L394	D395	R396	E397	S398	S399	E399	V400	Y401	K402	M403	M404	T405	T406	T407	V408	A408	A409	Z410	M410	L411	V412	T413	T414	D415	D416	V417	S418	V419	G420	T421	G422	T423	G424	T425	L426	L427	L428	H429	V430	L431	M432	D433	M434	D435	N436	G437	P438
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P440	S441	P442	R443	T446	M447	C448	D449	Q450	M451	P452	L457	T458	I459	S460	D461	I464	P465	P466	M467	T468	Y469	P470	Y471	K472	V473	S474	L475	S476	H477	G478	S479	D480	L481	T482	V483	K484	A485	E486	L487	D488	S489	K490	G491	T492	S493	M494	L495	L496	S497	P498	T499	Q500	Q501	L502	K503	S504
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[illegible]

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

ASN	ASN	VAL	VAL	PRO	THR	LEU	MET	PRO	ALA	ALA	HIS	PRO	TYR	ARG	ARG	PRO	SER	ASN	PRO	ASP	GLU	ILE	GLY	ASN	PHE	ILE	ASP	GLU	ASN	LEU	ASP	ALA	ALA	ASP	ASN	ASP	THR	THR	ALA	PRO	PRO	TYR	ASP	SER	LEU	LEU	VAL	PHE	ASP	TYR	GLY	GLY	SER	GLY	SER	GLU	GLU	ALA	ALA
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LEU	SER	SER	LEU	ASN	SER	SER	ASN	ASN	ASP	GLU	HIS	ASP	ASP	TYR	ASN	TYR	LEU	SER	ASP	TRP	GLY	SER	ARG	PHE	ARG	LYS	LEU	ALA	ASP	MET	TYR	GLY	GLY	ASP	ASP	ASP	GLU
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4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	no CTF correction. Imaging at underfocus 0.4 micron with CM200FEG microscope at 50,000 magnification	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	120000	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	500	Depositor
Magnification	68276	Depositor
Image detector	GATAN 794	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, NDG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.70	8/4276 (0.2%)	1.44	81/5839 (1.4%)
1	B	0.70	8/4276 (0.2%)	1.39	79/5839 (1.4%)
All	All	0.70	16/8552 (0.2%)	1.42	160/11678 (1.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	4
1	B	0	4
All	All	1	8

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	ALA	CA-CB	-8.37	1.34	1.52
1	B	335	ALA	CA-CB	-8.33	1.34	1.52
1	A	539	CYS	CB-SG	8.17	1.96	1.82
1	B	539	CYS	CB-SG	8.15	1.96	1.82
1	B	223	PRO	CG-CD	7.02	1.73	1.50
1	A	223	PRO	CG-CD	7.00	1.73	1.50
1	A	523	THR	N-CA	-6.26	1.33	1.46
1	B	523	THR	N-CA	-6.24	1.33	1.46
1	A	522	LEU	N-CA	-5.98	1.34	1.46
1	A	18	PRO	N-CD	5.97	1.56	1.47
1	B	522	LEU	N-CA	-5.97	1.34	1.46
1	B	18	PRO	N-CD	5.91	1.56	1.47
1	A	530	CYS	CB-SG	5.53	1.91	1.82
1	B	530	CYS	CB-SG	5.46	1.91	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	499	THR	CA-CB	5.05	1.66	1.53
1	B	499	THR	CA-CB	5.02	1.66	1.53

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	LYS	N-CA-CB	-28.44	59.41	110.60
1	A	520	PRO	CA-C-N	-13.30	87.95	117.20
1	B	520	PRO	CA-C-N	-13.28	87.99	117.20
1	B	290	PHE	N-CA-C	12.73	145.38	111.00
1	A	235	ILE	N-CA-C	12.72	145.34	111.00
1	B	235	ILE	N-CA-C	12.72	145.34	111.00
1	A	290	PHE	N-CA-C	12.71	145.32	111.00
1	B	374	ASP	N-CA-C	11.61	142.35	111.00
1	A	374	ASP	N-CA-C	11.61	142.34	111.00
1	A	17	PHE	C-N-CD	-11.55	95.19	120.60
1	B	17	PHE	C-N-CD	-11.54	95.22	120.60
1	B	398	SER	N-CA-C	11.37	141.70	111.00
1	A	398	SER	N-CA-C	11.36	141.68	111.00
1	B	465	PRO	C-N-CD	-11.04	96.31	120.60
1	A	465	PRO	C-N-CD	-11.03	96.33	120.60
1	B	222	ASP	CB-CG-OD2	10.06	127.35	118.30
1	A	222	ASP	CB-CG-OD2	10.03	127.33	118.30
1	A	236	GLY	N-CA-C	-9.99	88.11	113.10
1	B	236	GLY	N-CA-C	-9.98	88.15	113.10
1	A	230	VAL	C-N-CD	-9.94	98.73	120.60
1	B	230	VAL	C-N-CD	-9.92	98.77	120.60
1	A	374	ASP	CB-CA-C	-9.67	91.05	110.40
1	B	374	ASP	CB-CA-C	-9.66	91.08	110.40
1	B	376	ALA	N-CA-C	9.65	137.04	111.00
1	A	376	ALA	N-CA-C	9.64	137.04	111.00
1	B	522	LEU	CA-CB-CG	-9.38	93.74	115.30
1	A	522	LEU	CA-CB-CG	-9.36	93.77	115.30
1	B	223	PRO	N-CA-C	-9.30	87.91	112.10
1	B	520	PRO	N-CA-C	9.30	136.28	112.10
1	A	221	PHE	C-N-CA	-9.30	98.46	121.70
1	B	221	PHE	C-N-CA	-9.29	98.46	121.70
1	A	223	PRO	N-CA-C	-9.29	87.94	112.10
1	A	520	PRO	N-CA-C	9.29	136.25	112.10
1	B	481	LEU	N-CA-C	-9.29	85.92	111.00
1	A	481	LEU	N-CA-C	-9.27	85.97	111.00
1	B	481	LEU	CA-CB-CG	-8.76	95.16	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	LEU	CA-CB-CG	-8.75	95.17	115.30
1	A	289	ASP	C-N-CA	-8.43	100.62	121.70
1	B	289	ASP	C-N-CA	-8.42	100.66	121.70
1	A	516	ALA	N-CA-C	-8.35	88.47	111.00
1	B	516	ALA	N-CA-C	-8.35	88.46	111.00
1	B	222	ASP	C-N-CD	-8.21	102.54	120.60
1	A	290	PHE	CA-C-N	-8.20	99.16	117.20
1	B	290	PHE	CA-C-N	-8.19	99.18	117.20
1	A	222	ASP	C-N-CD	-8.19	102.59	120.60
1	A	46	PRO	C-N-CD	-8.05	102.89	120.60
1	B	46	PRO	C-N-CD	-8.03	102.93	120.60
1	B	233	ASN	N-CA-C	7.88	132.28	111.00
1	A	233	ASN	N-CA-C	7.86	132.22	111.00
1	A	336	VAL	N-CA-C	7.82	132.10	111.00
1	B	336	VAL	N-CA-C	7.81	132.09	111.00
1	B	522	LEU	C-N-CA	-7.79	102.21	121.70
1	A	522	LEU	C-N-CA	-7.78	102.25	121.70
1	B	362	GLN	N-CA-C	-7.71	90.18	111.00
1	A	362	GLN	N-CA-C	-7.71	90.20	111.00
1	A	234	GLU	N-CA-C	-7.59	90.51	111.00
1	B	234	GLU	N-CA-C	-7.58	90.52	111.00
1	A	234	GLU	C-N-CA	7.42	140.24	121.70
1	B	234	GLU	C-N-CA	7.41	140.22	121.70
1	A	521	GLN	C-N-CA	-7.38	103.25	121.70
1	B	521	GLN	C-N-CA	-7.38	103.26	121.70
1	A	490	LYS	CB-CA-C	7.32	125.04	110.40
1	B	277	SER	N-CA-C	-7.21	91.54	111.00
1	A	277	SER	N-CA-C	-7.20	91.56	111.00
1	A	337	SER	N-CA-C	-7.19	91.59	111.00
1	B	337	SER	N-CA-C	-7.16	91.67	111.00
1	B	503	LYS	N-CA-C	7.01	129.94	111.00
1	A	503	LYS	N-CA-C	7.00	129.91	111.00
1	B	523	THR	N-CA-CB	-6.95	97.10	110.30
1	A	523	THR	N-CA-CB	-6.93	97.13	110.30
1	A	492	THR	N-CA-C	6.78	129.30	111.00
1	B	492	THR	N-CA-C	6.75	129.23	111.00
1	B	448	CYS	CA-CB-SG	-6.70	101.95	114.00
1	A	448	CYS	CA-CB-SG	-6.68	101.98	114.00
1	A	398	SER	C-N-CA	-6.57	105.29	121.70
1	B	476	SER	N-CA-C	6.57	128.72	111.00
1	A	476	SER	N-CA-C	6.56	128.72	111.00
1	B	491	GLY	N-CA-C	6.55	129.47	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	398	SER	C-N-CA	-6.55	105.33	121.70
1	A	491	GLY	N-CA-C	6.53	129.43	113.10
1	B	525	VAL	N-CA-C	-6.50	93.46	111.00
1	A	525	VAL	N-CA-C	-6.48	93.50	111.00
1	A	335	ALA	N-CA-C	-6.32	93.95	111.00
1	B	335	ALA	N-CA-C	-6.31	93.96	111.00
1	B	532	CYS	N-CA-C	6.30	128.01	111.00
1	A	532	CYS	N-CA-C	6.30	128.00	111.00
1	B	234	GLU	CA-C-N	-6.28	103.38	117.20
1	A	234	GLU	CA-C-N	-6.28	103.39	117.20
1	A	222	ASP	N-CA-C	6.17	127.64	111.00
1	B	222	ASP	N-CA-C	6.15	127.61	111.00
1	A	235	ILE	CA-C-N	-6.14	103.91	116.20
1	A	397	GLU	C-N-CA	-6.14	106.35	121.70
1	B	235	ILE	CA-C-N	-6.13	103.94	116.20
1	B	397	GLU	C-N-CA	-6.12	106.40	121.70
1	A	18	PRO	CA-N-CD	-6.11	102.94	111.50
1	B	503	LYS	CB-CA-C	-6.09	98.21	110.40
1	A	503	LYS	CB-CA-C	-6.07	98.25	110.40
1	B	18	PRO	CA-N-CD	-6.07	103.00	111.50
1	B	502	LEU	N-CA-C	6.07	127.40	111.00
1	A	502	LEU	N-CA-C	6.04	127.31	111.00
1	A	2	TRP	N-CA-C	-6.03	94.72	111.00
1	B	2	TRP	N-CA-C	-6.01	94.77	111.00
1	B	374	ASP	C-N-CD	5.97	140.95	128.40
1	B	222	ASP	N-CA-CB	5.96	121.32	110.60
1	A	374	ASP	C-N-CD	5.95	140.90	128.40
1	A	222	ASP	N-CA-CB	5.95	121.31	110.60
1	A	364	ILE	N-CA-C	-5.93	95.00	111.00
1	B	364	ILE	N-CA-C	-5.93	95.00	111.00
1	B	376	ALA	CA-C-N	-5.85	104.33	117.20
1	A	376	ALA	CA-C-N	-5.83	104.36	117.20
1	A	382	ASN	N-CA-C	-5.83	95.27	111.00
1	B	382	ASN	N-CA-C	-5.81	95.31	111.00
1	B	471	TYR	N-CA-C	5.74	126.51	111.00
1	A	471	TYR	N-CA-C	5.73	126.46	111.00
1	A	481	LEU	CA-C-N	-5.67	104.72	117.20
1	B	481	LEU	CA-C-N	-5.67	104.72	117.20
1	A	374	ASP	C-N-CA	-5.67	98.20	122.00
1	B	374	ASP	C-N-CA	-5.67	98.20	122.00
1	B	403	ASN	N-CA-C	-5.63	95.81	111.00
1	A	403	ASN	N-CA-C	-5.62	95.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	PHE	CA-C-N	5.58	129.48	117.20
1	A	221	PHE	CA-C-N	5.57	129.46	117.20
1	A	505	GLY	N-CA-C	5.57	127.02	113.10
1	B	505	GLY	N-CA-C	5.54	126.96	113.10
1	B	502	LEU	CB-CA-C	-5.54	99.67	110.20
1	A	502	LEU	CB-CA-C	-5.52	99.71	110.20
1	A	157	GLU	C-N-CD	-5.48	108.54	120.60
1	B	157	GLU	C-N-CD	-5.47	108.57	120.60
1	B	519	ASN	N-CA-C	5.35	125.45	111.00
1	A	519	ASN	N-CA-C	5.35	125.44	111.00
1	A	405	THR	N-CA-C	5.33	125.40	111.00
1	B	405	THR	N-CA-C	5.32	125.35	111.00
1	A	367	LEU	CA-CB-CG	-5.31	103.08	115.30
1	B	367	LEU	CA-CB-CG	-5.29	103.12	115.30
1	A	521	GLN	N-CA-C	-5.21	96.93	111.00
1	B	521	GLN	N-CA-C	-5.21	96.94	111.00
1	A	290	PHE	O-C-N	5.19	131.01	122.70
1	A	532	CYS	N-CA-CB	-5.16	101.31	110.60
1	B	290	PHE	O-C-N	5.16	130.96	122.70
1	B	520	PRO	C-N-CA	5.15	134.58	121.70
1	B	532	CYS	N-CA-CB	-5.14	101.35	110.60
1	A	520	PRO	C-N-CA	5.13	134.54	121.70
1	A	18	PRO	CA-CB-CG	-5.13	94.25	104.00
1	B	522	LEU	N-CA-C	-5.12	97.17	111.00
1	A	522	LEU	N-CA-C	-5.11	97.19	111.00
1	B	18	PRO	CA-CB-CG	-5.11	94.28	104.00
1	A	339	VAL	N-CA-C	5.11	124.80	111.00
1	B	339	VAL	N-CA-C	5.10	124.77	111.00
1	B	16	PRO	C-N-CA	-5.09	108.98	121.70
1	A	16	PRO	C-N-CA	-5.07	109.02	121.70
1	A	332	PHE	N-CA-C	-5.04	97.39	111.00
1	B	234	GLU	O-C-N	5.03	130.75	122.70
1	B	332	PHE	N-CA-C	-5.03	97.43	111.00
1	A	470	PRO	N-CA-C	5.02	125.16	112.10
1	B	221	PHE	N-CA-C	5.02	124.56	111.00
1	A	539	CYS	N-CA-C	5.01	124.53	111.00
1	B	470	PRO	N-CA-C	5.01	125.13	112.10
1	B	539	CYS	N-CA-C	5.01	124.53	111.00
1	A	221	PHE	N-CA-C	5.01	124.52	111.00
1	A	234	GLU	O-C-N	5.00	130.71	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	490	LYS	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	PHE	Sidechain
1	A	18	PRO	Mainchain
1	A	222	ASP	Mainchain
1	A	520	PRO	Mainchain
1	B	17	PHE	Sidechain
1	B	18	PRO	Mainchain
1	B	222	ASP	Mainchain
1	B	520	PRO	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4191	0	4085	707	0
1	B	4191	0	4090	720	0
2	A	154	0	143	85	0
2	B	154	0	143	84	0
3	A	56	0	52	16	0
3	B	56	0	52	17	0
4	A	12	0	0	0	0
4	B	12	0	0	0	0
All	All	8826	0	8565	1392	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 80.

All (1392) 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:B:464:ILE:HD12	1:B:465:PRO:CD	1.30	1.58
1:A:464:ILE:HD12	1:A:465:PRO:CD	1.30	1.55
1:A:87:PRO:CG	1:B:89:GLU:HB3	1.16	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:ILE:CD1	1:B:465:PRO:HD2	1.50	1.41
1:A:464:ILE:CD1	1:A:465:PRO:HD2	1.50	1.37
1:A:87:PRO:CG	1:B:89:GLU:CB	2.03	1.36
1:A:82:SER:O	1:B:91:PRO:HD2	1.18	1.32
1:A:82:SER:OG	1:B:91:PRO:CB	1.79	1.28
1:A:31:PHE:HB2	1:B:93:GLU:OE2	1.08	1.25
1:A:82:SER:OG	1:B:91:PRO:HB2	1.12	1.23
1:B:540:GLN:O	1:B:540:GLN:CD	1.79	1.20
1:A:87:PRO:HG3	1:B:89:GLU:CB	1.66	1.19
1:A:540:GLN:CD	1:A:540:GLN:O	1.79	1.19
1:A:31:PHE:CB	1:B:93:GLU:OE2	1.90	1.18
1:B:450:GLN:HG2	1:B:532:CYS:O	1.43	1.18
1:A:84:ASN:HB2	1:B:79:HIS:CE1	1.77	1.17
1:A:423:THR:HB	2:A:810:NAG:C7	1.76	1.16
1:B:482:THR:HG23	1:B:499:THR:CG2	1.74	1.16
1:B:469:TYR:CG	1:B:470:PRO:HD2	1.81	1.16
1:A:482:THR:HG23	1:A:499:THR:CG2	1.75	1.15
1:B:234:GLU:H	1:B:235:ILE:HG23	1.08	1.15
1:A:450:GLN:HG2	1:A:532:CYS:O	1.44	1.15
1:A:474:SER:HB2	1:A:512:LEU:HG	1.25	1.15
1:A:8:LYS:HD2	1:A:8:LYS:H	1.04	1.15
1:A:469:TYR:CG	1:A:470:PRO:HD2	1.81	1.14
1:B:423:THR:HB	2:B:810:NAG:C7	1.76	1.13
1:B:8:LYS:HD2	1:B:8:LYS:H	1.04	1.13
1:B:301:THR:HG21	2:B:805:NAG:H82	1.29	1.12
1:B:154:ASP:C	2:B:801:NAG:H82	1.70	1.12
1:A:89:GLU:OE1	1:B:1:ASP:C	1.88	1.11
1:B:338:ARG:HD3	1:B:352:ILE:HG22	1.26	1.11
1:A:154:ASP:C	2:A:801:NAG:H82	1.70	1.10
1:B:222:ASP:O	1:B:222:ASP:OD1	1.69	1.10
1:B:227:THR:HG21	2:B:807:NAG:C8	1.82	1.10
1:A:32:ASN:HD21	1:A:83:GLU:HB2	0.98	1.10
1:A:227:THR:HG21	2:A:807:NAG:C8	1.82	1.09
1:A:234:GLU:H	1:A:235:ILE:HG23	1.08	1.09
1:A:301:THR:HG21	2:A:805:NAG:H82	1.29	1.09
1:A:222:ASP:OD1	1:A:222:ASP:O	1.69	1.09
1:A:90:GLU:O	1:B:1:ASP:OD1	1.70	1.08
1:A:338:ARG:HD3	1:A:352:ILE:HG22	1.26	1.07
1:A:482:THR:HG23	1:A:499:THR:HG22	1.09	1.07
1:A:485:ALA:O	1:A:486:GLU:HG2	1.54	1.07
1:B:32:ASN:HD21	1:B:83:GLU:HB2	0.98	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:GLN:CG	1:B:532:CYS:O	2.02	1.07
1:A:450:GLN:CG	1:A:532:CYS:O	2.03	1.07
1:B:485:ALA:O	1:B:486:GLU:HG2	1.54	1.07
1:B:464:ILE:CD1	1:B:465:PRO:CD	2.20	1.06
1:A:335:ALA:HB1	3:A:811:NDG:O6	1.54	1.06
1:B:474:SER:HB2	1:B:512:LEU:HG	1.25	1.06
1:A:290:PHE:HB2	1:A:292:LEU:N	1.69	1.06
1:B:335:ALA:HB1	3:B:811:NDG:O6	1.55	1.06
1:B:482:THR:HG23	1:B:499:THR:HG22	1.09	1.06
1:B:290:PHE:HB2	1:B:292:LEU:N	1.69	1.06
1:A:90:GLU:HB2	1:B:2:TRP:HB2	1.35	1.05
1:B:337:SER:HA	1:B:427:ILE:HG23	1.38	1.05
1:B:290:PHE:HB2	1:B:292:LEU:H	0.89	1.05
1:A:87:PRO:CD	1:B:89:GLU:HB3	1.86	1.05
1:A:84:ASN:CB	1:B:79:HIS:HE1	1.70	1.04
1:A:469:TYR:CD1	1:A:470:PRO:HD2	1.92	1.04
1:B:469:TYR:CD1	1:B:470:PRO:HD2	1.91	1.03
1:A:522:LEU:HD22	1:A:523:THR:HB	1.39	1.03
1:A:464:ILE:CD1	1:A:465:PRO:CD	2.20	1.03
1:B:522:LEU:HD22	1:B:523:THR:HB	1.39	1.03
1:B:482:THR:CG2	1:B:499:THR:N	2.22	1.03
1:A:84:ASN:HB2	1:B:79:HIS:HE1	0.91	1.03
1:A:482:THR:CG2	1:A:499:THR:N	2.22	1.02
1:A:432:ASP:OD2	1:A:464:ILE:HG22	1.60	1.02
1:A:482:THR:HG21	1:A:499:THR:H	1.23	1.02
1:B:432:ASP:OD2	1:B:464:ILE:HG22	1.60	1.02
1:B:403:ASN:HB2	3:B:902:NDG:C8	1.90	1.02
1:A:403:ASN:HB2	3:A:902:NDG:C8	1.90	1.01
1:B:450:GLN:HB2	1:B:533:GLU:HA	1.41	1.01
1:A:337:SER:HA	1:A:427:ILE:HG23	1.38	1.01
1:B:274:ASP:O	1:B:278:ASN:HA	1.61	1.01
1:A:450:GLN:HB2	1:A:533:GLU:HA	1.41	1.01
1:B:188:THR:HG23	1:B:208:ILE:HG12	1.43	1.00
1:A:82:SER:HG	1:B:91:PRO:CB	1.61	1.00
1:A:290:PHE:HB2	1:A:292:LEU:H	0.88	1.00
1:A:274:ASP:O	1:A:278:ASN:HA	1.61	1.00
1:A:188:THR:HG23	1:A:208:ILE:HG12	1.43	0.99
1:A:482:THR:CG2	1:A:499:THR:H	1.76	0.99
1:A:523:THR:HG23	1:A:524:VAL:H	1.26	0.99
1:B:523:THR:HG23	1:B:524:VAL:H	1.26	0.99
1:B:366:LYS:HG3	1:B:367:LEU:H	1.28	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:THR:HG21	1:B:499:THR:H	1.23	0.99
1:B:320:THR:HG21	2:B:807:NAG:N2	1.78	0.98
1:A:320:THR:HG21	2:A:807:NAG:N2	1.78	0.98
1:A:82:SER:O	1:B:91:PRO:CD	2.12	0.97
1:B:482:THR:CG2	1:B:499:THR:H	1.76	0.97
1:A:8:LYS:CD	1:A:8:LYS:H	1.74	0.97
1:A:366:LYS:HG3	1:A:367:LEU:H	1.28	0.96
1:A:235:ILE:CG1	1:A:287:GLY:HA2	1.96	0.96
1:A:32:ASN:HD21	1:A:83:GLU:CB	1.79	0.96
1:B:8:LYS:H	1:B:8:LYS:CD	1.74	0.96
1:B:235:ILE:CG1	1:B:287:GLY:HA2	1.96	0.96
1:B:32:ASN:HD21	1:B:83:GLU:CB	1.79	0.96
1:B:227:THR:HG21	2:B:807:NAG:H83	1.48	0.96
1:A:290:PHE:CB	1:A:292:LEU:H	1.79	0.95
1:A:366:LYS:CG	1:A:367:LEU:H	1.80	0.94
1:A:82:SER:OG	1:B:91:PRO:CA	2.14	0.94
1:A:227:THR:HG21	2:A:807:NAG:H83	1.48	0.94
1:B:366:LYS:CG	1:B:367:LEU:H	1.80	0.94
1:B:290:PHE:CB	1:B:292:LEU:H	1.79	0.93
1:A:289:ASP:O	1:A:290:PHE:HB3	1.67	0.93
1:A:482:THR:HG21	1:A:499:THR:N	1.81	0.93
1:A:32:ASN:ND2	1:A:83:GLU:HB2	1.84	0.93
1:A:396:ARG:HH22	1:A:464:ILE:HB	1.33	0.93
1:B:464:ILE:HD12	1:B:465:PRO:HD2	0.94	0.93
1:B:289:ASP:O	1:B:290:PHE:HB3	1.67	0.93
1:A:195:ASP:HB2	1:A:201:LEU:H	1.34	0.92
2:A:805:NAG:H62	2:A:806:NAG:C7	2.00	0.92
1:B:27:ASN:HD22	1:B:28:LYS:N	1.66	0.92
1:A:87:PRO:HG2	1:B:89:GLU:CB	2.00	0.92
1:A:87:PRO:HG2	1:B:89:GLU:HB3	1.49	0.92
1:A:446:THR:HG23	1:A:539:CYS:SG	2.09	0.92
1:B:320:THR:HG21	2:B:807:NAG:HN2	1.31	0.92
1:A:335:ALA:CB	3:A:811:NDG:O6	2.18	0.92
1:B:446:THR:HG23	1:B:539:CYS:SG	2.09	0.92
1:A:27:ASN:HD22	1:A:28:LYS:N	1.66	0.92
1:A:352:ILE:HG13	1:A:388:VAL:HB	1.51	0.92
1:B:403:ASN:HB2	3:B:902:NDG:C7	2.00	0.92
1:A:227:THR:HG21	2:A:807:NAG:C7	1.99	0.92
1:A:517:GLN:O	1:A:519:ASN:N	2.03	0.91
1:B:227:THR:HG21	2:B:807:NAG:C7	1.99	0.91
1:B:32:ASN:ND2	1:B:83:GLU:HB2	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ASP:HB2	1:B:201:LEU:H	1.34	0.91
1:B:464:ILE:HD12	1:B:465:PRO:HD3	1.53	0.91
1:A:404:ASN:ND2	1:A:404:ASN:O	2.03	0.91
1:A:403:ASN:HB2	3:A:902:NDG:C7	2.00	0.91
2:B:805:NAG:H62	2:B:806:NAG:C7	1.99	0.91
1:B:396:ARG:HH22	1:B:464:ILE:HB	1.33	0.91
1:B:335:ALA:CB	3:B:811:NDG:O6	2.18	0.91
1:A:320:THR:HG21	2:A:807:NAG:HN2	1.31	0.91
2:A:805:NAG:O5	2:A:806:NAG:H83	1.71	0.91
1:B:352:ILE:HG13	1:B:388:VAL:HB	1.51	0.91
1:A:90:GLU:HB2	1:B:2:TRP:CB	2.00	0.90
1:B:404:ASN:ND2	1:B:404:ASN:O	2.03	0.90
1:A:464:ILE:HD12	1:A:465:PRO:HD2	0.94	0.90
1:B:518:ASN:O	1:B:520:PRO:HD3	1.72	0.90
1:A:340:ASP:HA	1:A:429:HIS:HB3	1.53	0.90
1:A:378:TRP:HB2	1:A:379:LEU:HD23	1.53	0.90
1:A:234:GLU:N	1:A:235:ILE:HG23	1.86	0.90
1:B:482:THR:HG21	1:B:499:THR:N	1.81	0.90
2:B:805:NAG:O5	2:B:806:NAG:H83	1.71	0.90
1:A:518:ASN:O	1:A:520:PRO:HD3	1.72	0.90
1:B:396:ARG:NH2	1:B:464:ILE:CG2	2.35	0.90
1:B:517:GLN:O	1:B:519:ASN:N	2.03	0.90
1:A:374:ASP:O	1:A:375:PRO:C	2.06	0.89
1:A:396:ARG:NH2	1:A:464:ILE:CG2	2.35	0.89
1:A:464:ILE:HD11	1:A:465:PRO:HD2	1.53	0.89
1:B:374:ASP:O	1:B:375:PRO:C	2.06	0.89
1:B:234:GLU:N	1:B:235:ILE:HG23	1.86	0.89
1:A:523:THR:HG23	1:A:524:VAL:CG2	2.03	0.89
1:A:371:ILE:CD1	1:A:381:VAL:HG11	2.03	0.89
1:A:449:ASP:H	1:A:532:CYS:HB3	1.37	0.89
1:B:338:ARG:HD3	1:B:352:ILE:CG2	2.02	0.89
1:B:464:ILE:HD11	1:B:465:PRO:HD2	1.53	0.89
1:B:154:ASP:HB3	1:B:155:PRO:HD2	1.54	0.89
1:B:523:THR:HG23	1:B:524:VAL:CG2	2.03	0.89
1:A:8:LYS:HD2	1:A:8:LYS:N	1.87	0.89
1:B:8:LYS:HD2	1:B:8:LYS:N	1.87	0.88
1:B:371:ILE:CD1	1:B:381:VAL:HG11	2.03	0.88
1:A:338:ARG:HD3	1:A:352:ILE:CG2	2.02	0.88
1:B:340:ASP:HA	1:B:429:HIS:HB3	1.53	0.88
1:B:449:ASP:H	1:B:532:CYS:HB3	1.37	0.88
1:A:343:GLU:HB3	1:A:433:VAL:HG21	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ALA:O	1:B:273:THR:HG21	1.74	0.88
1:B:378:TRP:HB2	1:B:379:LEU:HD23	1.53	0.88
1:A:221:PHE:HE1	1:A:315:SER:O	1.56	0.87
1:A:87:PRO:CD	1:B:89:GLU:CB	2.46	0.87
1:B:483:TRP:CZ3	1:B:498:PRO:HG3	2.09	0.87
1:A:154:ASP:HB3	1:A:155:PRO:HD2	1.54	0.87
1:A:318:THR:HG21	2:A:806:NAG:H5	1.56	0.87
1:A:333:VAL:HB	1:A:334:PRO:HD3	1.56	0.87
1:A:464:ILE:HD12	1:A:465:PRO:HD3	1.53	0.87
1:A:441:SER:OG	1:A:442:PRO:HD3	1.75	0.87
1:B:441:SER:OG	1:B:442:PRO:HD3	1.75	0.87
1:B:320:THR:HG21	2:B:807:NAG:C2	2.05	0.87
1:A:257:ALA:O	1:A:273:THR:HG21	1.74	0.86
1:A:440:PRO:CD	1:A:522:LEU:HD12	2.05	0.86
1:A:320:THR:HG21	2:A:807:NAG:C2	2.05	0.86
1:B:318:THR:HG21	2:B:806:NAG:H5	1.56	0.86
1:A:483:TRP:CZ3	1:A:498:PRO:HG3	2.09	0.86
1:A:523:THR:HG23	1:A:524:VAL:N	1.90	0.86
1:B:486:GLU:HB2	1:B:495:LEU:HB2	1.56	0.86
1:A:82:SER:HG	1:B:91:PRO:HB2	0.90	0.86
1:B:343:GLU:HB3	1:B:433:VAL:HG21	1.55	0.86
1:A:486:GLU:HB2	1:A:495:LEU:HB2	1.56	0.86
1:B:423:THR:CB	2:B:810:NAG:C7	2.54	0.86
1:B:221:PHE:HE1	1:B:315:SER:O	1.56	0.86
1:A:90:GLU:CB	1:B:2:TRP:HB2	2.06	0.86
1:B:333:VAL:HB	1:B:334:PRO:HD3	1.56	0.86
1:A:235:ILE:HG13	1:A:287:GLY:HA2	1.58	0.85
1:B:438:PRO:HB3	1:B:471:TYR:HE2	1.41	0.85
1:B:440:PRO:CD	1:B:522:LEU:HD12	2.05	0.85
1:A:423:THR:CB	2:A:810:NAG:C7	2.54	0.85
1:B:451:ASN:N	1:B:533:GLU:O	2.10	0.85
1:A:464:ILE:HD12	1:A:465:PRO:N	1.91	0.85
1:A:483:TRP:HZ2	1:A:507:TYR:CE1	1.95	0.85
1:B:464:ILE:HD12	1:B:465:PRO:N	1.91	0.85
1:A:375:PRO:HB3	1:A:400:TYR:CE2	2.12	0.85
1:B:483:TRP:HZ2	1:B:507:TYR:CE1	1.95	0.85
1:A:87:PRO:HG2	1:B:89:GLU:CG	2.06	0.84
1:B:483:TRP:HZ2	1:B:507:TYR:HE1	1.24	0.84
1:A:440:PRO:HD2	1:A:522:LEU:HD12	1.59	0.84
1:B:523:THR:HG23	1:B:524:VAL:N	1.90	0.84
1:A:483:TRP:HZ2	1:A:507:TYR:HE1	1.24	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLU:OE2	1:B:3:VAL:HG13	1.76	0.84
1:B:235:ILE:HG13	1:B:287:GLY:HA2	1.58	0.84
1:A:230:VAL:O	1:A:324:GLU:N	2.11	0.84
1:A:396:ARG:NE	1:A:432:ASP:HB2	1.93	0.83
1:A:451:ASN:N	1:A:533:GLU:O	2.10	0.83
1:A:469:TYR:CG	1:A:470:PRO:CD	2.61	0.83
1:B:375:PRO:HB3	1:B:400:TYR:CE2	2.12	0.83
1:A:423:THR:HB	2:A:810:NAG:N2	1.93	0.83
1:B:147:SER:OG	1:B:167:ARG:HD2	1.78	0.83
1:A:155:PRO:HB2	2:A:801:NAG:H81	1.59	0.83
1:A:32:ASN:ND2	1:A:83:GLU:H	1.77	0.83
1:B:230:VAL:O	1:B:324:GLU:N	2.11	0.83
1:B:440:PRO:HD2	1:B:522:LEU:HD12	1.59	0.83
1:A:423:THR:CB	2:A:810:NAG:N2	2.42	0.83
1:A:234:GLU:H	1:A:235:ILE:CG2	1.92	0.83
1:A:289:ASP:OD2	1:A:289:ASP:O	1.97	0.83
1:A:89:GLU:OE1	1:B:1:ASP:CA	2.09	0.83
1:B:289:ASP:OD2	1:B:289:ASP:O	1.97	0.83
1:B:396:ARG:NE	1:B:432:ASP:HB2	1.93	0.83
1:A:87:PRO:HD3	1:B:89:GLU:HB2	1.61	0.83
1:B:423:THR:HB	2:B:810:NAG:N2	1.93	0.83
1:B:448:CYS:O	1:B:452:PRO:HG3	1.79	0.83
1:A:448:CYS:O	1:A:452:PRO:HG3	1.79	0.82
1:A:438:PRO:HB3	1:A:471:TYR:HE2	1.41	0.82
1:B:28:LYS:HD3	1:B:88:VAL:HG12	1.61	0.82
1:B:32:ASN:ND2	1:B:83:GLU:H	1.77	0.82
1:B:423:THR:CB	2:B:810:NAG:N2	2.42	0.82
1:A:540:GLN:OE1	1:A:540:GLN:O	1.97	0.82
1:B:154:ASP:HB3	2:B:801:NAG:HN2	1.45	0.82
1:A:87:PRO:HD3	1:B:89:GLU:CB	2.10	0.82
1:A:154:ASP:HB3	2:A:801:NAG:N2	1.95	0.82
1:B:155:PRO:HB2	2:B:801:NAG:H81	1.59	0.82
1:A:154:ASP:HB3	2:A:801:NAG:HN2	1.44	0.82
1:B:482:THR:HG21	1:B:500:GLN:N	1.94	0.82
1:B:154:ASP:HB3	2:B:801:NAG:N2	1.95	0.81
1:A:446:THR:HG21	1:A:537:ILE:O	1.79	0.81
1:B:469:TYR:CG	1:B:470:PRO:CD	2.61	0.81
1:B:299:GLN:HG2	1:B:318:THR:HG23	1.63	0.81
1:B:290:PHE:CE2	1:B:293:ARG:HB2	2.16	0.81
1:A:469:TYR:CD2	1:A:470:PRO:HD2	2.16	0.81
1:A:482:THR:HG21	1:A:500:GLN:N	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:THR:HG21	1:B:537:ILE:O	1.79	0.81
1:A:265:GLU:HB3	1:A:268:PHE:HE2	1.46	0.81
1:A:486:GLU:O	1:A:494:MET:HA	1.81	0.81
1:B:265:GLU:HB3	1:B:268:PHE:HE2	1.46	0.81
1:A:290:PHE:CE2	1:A:293:ARG:HB2	2.16	0.81
1:A:517:GLN:C	1:A:519:ASN:H	1.84	0.81
1:B:277:SER:C	1:B:278:ASN:HD22	1.83	0.81
1:A:396:ARG:HH21	1:A:464:ILE:HG22	1.46	0.80
1:B:290:PHE:HD2	1:B:293:ARG:H	1.28	0.80
1:A:299:GLN:HG2	1:A:318:THR:HG23	1.62	0.80
1:B:540:GLN:OE1	1:B:540:GLN:O	1.97	0.80
1:A:432:ASP:OD2	1:A:464:ILE:CG2	2.30	0.80
1:A:84:ASN:CG	1:B:77:SER:OG	2.19	0.80
1:A:28:LYS:HD3	1:A:88:VAL:HG12	1.61	0.80
1:B:432:ASP:OD2	1:B:464:ILE:CG2	2.30	0.80
1:B:517:GLN:C	1:B:519:ASN:H	1.84	0.80
1:B:486:GLU:O	1:B:494:MET:HA	1.81	0.80
1:A:365:GLN:HG3	1:A:365:GLN:O	1.82	0.80
1:B:469:TYR:CD2	1:B:470:PRO:HD2	2.16	0.80
1:B:396:ARG:HD3	1:B:431:LEU:C	2.02	0.79
1:A:82:SER:C	1:B:91:PRO:HD2	2.01	0.79
1:A:127:VAL:HG13	1:A:128:MET:H	1.46	0.79
1:A:27:ASN:HD22	1:A:27:ASN:C	1.85	0.79
1:A:290:PHE:HD2	1:A:293:ARG:H	1.28	0.79
1:B:540:GLN:CG	1:B:540:GLN:O	2.31	0.79
1:B:195:ASP:HB3	1:B:200:GLY:HA3	1.65	0.79
1:B:482:THR:OG1	1:B:500:GLN:HG2	1.82	0.79
1:B:232:GLU:HG3	1:B:290:PHE:N	1.98	0.79
1:B:523:THR:CG2	1:B:524:VAL:H	1.94	0.79
1:A:496:LEU:HD21	1:A:509:ILE:HD13	1.63	0.79
1:B:27:ASN:HD22	1:B:27:ASN:C	1.85	0.79
1:B:496:LEU:HD21	1:B:509:ILE:HD13	1.63	0.79
2:B:904:NAG:H3	2:B:904:NAG:O7	1.82	0.79
1:A:195:ASP:HB3	1:A:200:GLY:HA3	1.65	0.79
1:A:485:ALA:O	1:A:486:GLU:CG	2.30	0.79
1:A:449:ASP:HB3	1:A:532:CYS:H	1.47	0.79
1:B:127:VAL:HG13	1:B:128:MET:H	1.46	0.79
1:A:406:TYR:CD1	2:A:808:NAG:H83	2.17	0.79
1:B:234:GLU:H	1:B:235:ILE:CG2	1.92	0.79
1:B:365:GLN:O	1:B:365:GLN:HG3	1.82	0.79
1:A:222:ASP:C	1:A:222:ASP:OD1	2.20	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:SER:C	1:A:278:ASN:HD22	1.84	0.79
1:A:155:PRO:C	1:A:157:GLU:H	1.86	0.78
1:A:156:GLU:HG3	1:A:160:PRO:HB3	1.66	0.78
1:A:396:ARG:HD3	1:A:431:LEU:C	2.03	0.78
1:B:396:ARG:HH21	1:B:464:ILE:HG22	1.46	0.78
1:A:482:THR:OG1	1:A:500:GLN:HG2	1.82	0.78
1:B:155:PRO:C	1:B:157:GLU:H	1.86	0.78
1:B:147:SER:OG	1:B:167:ARG:CG	2.32	0.78
1:B:485:ALA:O	1:B:486:GLU:CG	2.30	0.78
1:B:406:TYR:CD1	2:B:808:NAG:H83	2.17	0.78
2:B:809:NAG:H61	2:B:810:NAG:H62	1.65	0.78
2:A:904:NAG:O7	2:A:904:NAG:H3	1.82	0.78
1:B:147:SER:OG	1:B:167:ARG:CD	2.32	0.78
1:A:154:ASP:CB	1:A:155:PRO:HD2	2.13	0.78
1:A:371:ILE:HD11	1:A:381:VAL:HG11	1.64	0.78
1:B:371:ILE:HD11	1:B:381:VAL:HG11	1.64	0.78
1:A:89:GLU:OE1	1:B:2:TRP:N	2.18	0.77
1:A:290:PHE:HZ	1:A:296:TYR:HH	1.31	0.77
1:A:432:ASP:CG	1:A:464:ILE:HG22	2.05	0.77
1:B:154:ASP:CB	1:B:155:PRO:HD2	2.13	0.77
1:B:524:VAL:CG2	2:B:904:NAG:H81	2.14	0.77
1:A:232:GLU:HG3	1:A:290:PHE:N	1.98	0.77
1:A:540:GLN:CG	1:A:540:GLN:O	2.30	0.77
1:B:501:GLN:HG2	1:B:501:GLN:O	1.84	0.77
1:A:523:THR:CG2	1:A:524:VAL:N	2.46	0.77
1:A:89:GLU:CD	1:B:1:ASP:H3	1.86	0.77
1:B:301:THR:HG21	2:B:805:NAG:C8	2.12	0.77
1:B:523:THR:HG23	1:B:524:VAL:HG22	1.67	0.77
1:A:301:THR:HG21	2:A:805:NAG:C8	2.12	0.77
1:A:505:GLY:C	1:A:506:ASP:OD1	2.23	0.77
2:A:809:NAG:H61	2:A:810:NAG:H62	1.65	0.77
1:B:222:ASP:OD1	1:B:222:ASP:C	2.20	0.77
1:B:505:GLY:C	1:B:506:ASP:OD1	2.23	0.77
1:B:362:GLN:O	1:B:364:ILE:HG23	1.85	0.77
1:B:194:THR:HB	1:B:198:GLY:HA2	1.66	0.77
1:B:449:ASP:HB3	1:B:532:CYS:H	1.47	0.77
1:A:238:GLU:HA	1:A:283:THR:HG22	1.66	0.76
1:B:223:PRO:HD2	1:B:226:TYR:OH	1.85	0.76
1:B:238:GLU:HA	1:B:283:THR:HG22	1.66	0.76
1:B:432:ASP:CG	1:B:464:ILE:HG22	2.05	0.76
1:A:524:VAL:CG2	2:A:904:NAG:H81	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:THR:HG22	1:A:273:THR:H	1.51	0.76
1:A:366:LYS:CG	1:A:367:LEU:N	2.48	0.76
1:B:156:GLU:HG3	1:B:160:PRO:HB3	1.66	0.76
1:A:194:THR:HB	1:A:198:GLY:HA2	1.66	0.76
1:A:501:GLN:O	1:A:501:GLN:HG2	1.84	0.76
1:B:188:THR:HG23	1:B:208:ILE:CG1	2.16	0.76
1:A:362:GLN:O	1:A:364:ILE:HG23	1.85	0.76
1:B:523:THR:CG2	1:B:524:VAL:N	2.46	0.76
1:A:188:THR:HG23	1:A:208:ILE:CG1	2.16	0.75
1:A:371:ILE:HD12	1:A:410:MET:HB3	1.68	0.75
1:A:241:ARG:HE	1:A:281:ILE:HD12	1.51	0.75
1:A:289:ASP:O	1:A:290:PHE:CB	2.25	0.75
1:A:448:CYS:SG	1:A:537:ILE:HG22	2.27	0.75
1:A:523:THR:HG23	1:A:524:VAL:HG22	1.67	0.75
1:B:290:PHE:CD2	1:B:293:ARG:N	2.55	0.75
1:B:440:PRO:HB3	1:B:457:LEU:HD21	1.68	0.75
1:A:440:PRO:HB3	1:A:457:LEU:HD21	1.67	0.75
1:A:196:LEU:HB2	1:A:199:ALA:HB3	1.67	0.75
1:A:90:GLU:HB3	1:B:2:TRP:HD1	1.52	0.75
1:B:196:LEU:HB2	1:B:199:ALA:HB3	1.67	0.75
1:A:223:PRO:HD2	1:A:226:TYR:OH	1.85	0.75
1:B:272:THR:HG22	1:B:273:THR:H	1.51	0.75
1:B:290:PHE:HZ	1:B:296:TYR:HH	1.33	0.75
1:A:87:PRO:HG3	1:B:89:GLU:HB3	0.75	0.75
1:B:396:ARG:NH2	1:B:464:ILE:HB	2.02	0.75
1:A:396:ARG:NH2	1:A:464:ILE:HB	2.02	0.75
1:A:90:GLU:C	1:B:1:ASP:OD1	2.26	0.75
1:B:449:ASP:HB3	1:B:532:CYS:N	2.02	0.75
1:A:84:ASN:HD22	1:B:79:HIS:CE1	2.04	0.75
1:B:450:GLN:HG3	1:B:533:GLU:OE2	1.87	0.74
1:A:449:ASP:HB3	1:A:532:CYS:N	2.02	0.74
1:B:241:ARG:HE	1:B:281:ILE:HD12	1.51	0.74
1:B:448:CYS:SG	1:B:537:ILE:HG22	2.27	0.74
1:A:450:GLN:HG3	1:A:533:GLU:OE2	1.88	0.74
1:B:364:ILE:HG13	1:B:364:ILE:O	1.87	0.74
1:A:396:ARG:HH21	1:A:464:ILE:CG2	1.99	0.74
1:A:364:ILE:HG13	1:A:364:ILE:O	1.86	0.74
1:B:366:LYS:CG	1:B:367:LEU:N	2.48	0.74
1:B:223:PRO:HB2	1:B:226:TYR:CE2	2.23	0.74
1:B:298:LEU:HD23	1:B:298:LEU:N	2.03	0.74
1:A:87:PRO:HG2	1:B:89:GLU:HG3	1.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:ASN:O	1:B:534:GLY:HA2	1.88	0.73
1:A:290:PHE:HE2	1:A:293:ARG:HB2	1.52	0.73
1:B:371:ILE:HD12	1:B:410:MET:HB3	1.68	0.73
1:A:223:PRO:HB2	1:A:226:TYR:CE2	2.23	0.73
1:A:333:VAL:CB	1:A:334:PRO:HD3	2.18	0.73
1:A:373:ASN:ND2	1:A:374:ASP:H	1.87	0.73
1:B:373:ASN:ND2	1:B:374:ASP:H	1.87	0.73
1:A:276:GLU:HG3	1:A:277:SER:H	1.54	0.73
1:A:474:SER:CB	1:A:512:LEU:HG	2.14	0.73
1:A:273:THR:O	2:A:803:NAG:H82	1.89	0.73
1:B:333:VAL:CB	1:B:334:PRO:HD3	2.18	0.73
1:B:33:LYS:HB3	1:B:83:GLU:HG2	1.71	0.73
1:A:320:THR:CG2	2:A:807:NAG:N2	2.52	0.72
1:B:396:ARG:HH21	1:B:464:ILE:CG2	1.98	0.72
1:B:273:THR:O	2:B:803:NAG:H82	1.89	0.72
1:A:35:TYR:HB3	1:B:90:GLU:OE1	1.89	0.72
1:B:320:THR:CG2	2:B:807:NAG:N2	2.52	0.72
1:A:298:LEU:HD23	1:A:298:LEU:N	2.03	0.72
1:A:451:ASN:O	1:A:534:GLY:HA2	1.88	0.72
1:A:511:VAL:HG23	1:A:523:THR:O	1.89	0.72
1:A:342:SER:HA	1:A:431:LEU:HB2	1.71	0.72
1:B:342:SER:HA	1:B:431:LEU:HB2	1.71	0.72
1:A:87:PRO:CG	1:B:89:GLU:CG	2.67	0.72
1:B:276:GLU:HG3	1:B:277:SER:H	1.54	0.72
1:B:276:GLU:CG	1:B:277:SER:H	2.03	0.72
1:B:366:LYS:HG3	1:B:367:LEU:N	2.04	0.72
1:B:394:LEU:HD12	1:B:394:LEU:N	2.05	0.72
1:A:33:LYS:HB3	1:A:83:GLU:HG2	1.71	0.72
1:B:474:SER:CB	1:B:512:LEU:HG	2.14	0.72
1:A:405:THR:OG1	1:A:406:TYR:N	2.22	0.71
1:A:90:GLU:HB3	1:B:2:TRP:CD1	2.25	0.71
1:A:28:LYS:NZ	1:B:4:ILE:H	1.87	0.71
1:A:364:ILE:O	1:A:364:ILE:CG1	2.37	0.71
1:A:482:THR:CG2	1:A:499:THR:CG2	2.62	0.71
1:A:227:THR:O	2:A:812:NAG:O5	2.09	0.71
1:B:511:VAL:HG23	1:B:523:THR:O	1.89	0.71
1:A:276:GLU:CG	1:A:277:SER:H	2.03	0.71
1:A:320:THR:CG2	2:A:807:NAG:HN2	2.02	0.71
1:A:394:LEU:N	1:A:394:LEU:HD12	2.05	0.71
1:B:364:ILE:CG1	1:B:364:ILE:O	2.37	0.71
1:A:434:ASN:OD1	1:A:467:ASN:HB3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:THR:O	2:B:812:NAG:O5	2.09	0.71
1:B:414:ASP:HB3	1:B:420:GLY:HA3	1.73	0.71
1:B:229:LEU:HD23	1:B:322:THR:HB	1.73	0.71
1:A:290:PHE:CD2	1:A:293:ARG:N	2.55	0.71
1:A:474:SER:HB2	1:A:512:LEU:CG	2.15	0.71
1:B:316:THR:O	2:B:806:NAG:H82	1.91	0.71
1:A:368:SER:HG	1:A:370:PHE:HE1	1.39	0.71
1:A:438:PRO:HB3	1:A:471:TYR:CE2	2.26	0.71
1:A:187:TYR:HA	2:A:801:NAG:C7	2.21	0.71
1:A:366:LYS:HG3	1:A:367:LEU:N	2.04	0.70
1:A:414:ASP:HB3	1:A:420:GLY:HA3	1.73	0.70
1:B:290:PHE:HE2	1:B:293:ARG:HB2	1.52	0.70
1:B:403:ASN:CB	3:B:902:NDG:N2	2.54	0.70
1:B:434:ASN:OD1	1:B:467:ASN:HB3	1.90	0.70
1:B:482:THR:CG2	1:B:499:THR:CG2	2.62	0.70
1:B:438:PRO:HB3	1:B:471:TYR:CE2	2.26	0.70
1:A:316:THR:O	2:A:806:NAG:H82	1.91	0.70
1:B:187:TYR:HA	2:B:801:NAG:C7	2.21	0.70
1:A:403:ASN:CB	3:A:902:NDG:N2	2.54	0.70
1:B:320:THR:CG2	2:B:807:NAG:HN2	2.02	0.70
1:B:337:SER:CA	1:B:427:ILE:HG23	2.20	0.70
1:B:485:ALA:C	1:B:486:GLU:HG2	2.11	0.70
1:B:523:THR:HG23	1:B:524:VAL:HG23	1.74	0.70
1:A:289:ASP:CG	1:A:289:ASP:O	2.29	0.69
1:A:523:THR:HG23	1:A:524:VAL:HG23	1.74	0.69
1:A:229:LEU:HD23	1:A:322:THR:HB	1.73	0.69
1:A:485:ALA:C	1:A:486:GLU:HG2	2.11	0.69
1:A:53:ILE:HG13	1:A:59:TRP:O	1.93	0.69
1:B:27:ASN:ND2	1:B:27:ASN:C	2.46	0.69
1:B:186:GLU:OE1	2:B:801:NAG:H62	1.93	0.69
1:B:289:ASP:O	1:B:289:ASP:CG	2.30	0.69
1:B:483:TRP:CZ2	1:B:507:TYR:HE1	2.09	0.69
1:B:396:ARG:HE	1:B:432:ASP:HB2	1.57	0.69
1:A:27:ASN:C	1:A:27:ASN:ND2	2.46	0.69
1:B:289:ASP:O	1:B:290:PHE:CB	2.25	0.69
1:B:53:ILE:HG13	1:B:59:TRP:O	1.93	0.69
1:A:396:ARG:HE	1:A:432:ASP:HB2	1.57	0.69
1:A:186:GLU:OE1	2:A:801:NAG:H62	1.93	0.69
1:B:242:LEU:HD12	1:B:280:GLY:O	1.93	0.69
1:B:396:ARG:HD3	1:B:431:LEU:O	1.93	0.69
1:A:337:SER:CA	1:A:427:ILE:HG23	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:ASP:CG	1:B:2:TRP:H	1.96	0.68
1:B:282:LEU:HD23	1:B:283:THR:N	2.08	0.68
1:A:242:LEU:HD12	1:A:280:GLY:O	1.93	0.68
1:B:272:THR:HG22	1:B:273:THR:N	2.09	0.68
1:B:290:PHE:HZ	1:B:296:TYR:OH	1.77	0.68
1:B:396:ARG:HE	1:B:432:ASP:CB	2.07	0.68
1:A:282:LEU:HD23	1:A:283:THR:H	1.59	0.68
1:A:347:ARG:CD	1:A:392:GLY:H	2.07	0.68
1:B:155:PRO:HB2	2:B:801:NAG:C8	2.24	0.68
1:B:347:ARG:CD	1:B:392:GLY:H	2.07	0.68
1:A:282:LEU:HD23	1:A:283:THR:N	2.08	0.68
1:B:440:PRO:HA	1:B:458:THR:O	1.94	0.68
1:A:137:ASP:OD2	1:A:139:ILE:HG22	1.94	0.67
1:A:272:THR:HG22	1:A:273:THR:N	2.09	0.67
1:A:155:PRO:HB2	2:A:801:NAG:C8	2.24	0.67
1:A:482:THR:HG21	1:A:500:GLN:H	1.58	0.67
1:B:396:ARG:NH2	1:B:464:ILE:CB	2.58	0.67
1:A:232:GLU:HG2	1:A:289:ASP:HA	1.77	0.67
1:A:371:ILE:CG2	1:A:372:GLY:N	2.57	0.67
1:B:232:GLU:HG2	1:B:289:ASP:HA	1.77	0.67
1:B:371:ILE:CG2	1:B:372:GLY:N	2.57	0.67
1:B:401:VAL:HG13	1:B:405:THR:O	1.95	0.67
1:A:1:ASP:CG	1:A:2:TRP:H	1.96	0.67
3:A:902:NDG:O7	3:A:902:NDG:H3	1.95	0.67
1:B:333:VAL:HB	1:B:334:PRO:CD	2.24	0.67
1:B:347:ARG:CG	1:B:392:GLY:H	2.08	0.67
1:A:347:ARG:CG	1:A:392:GLY:H	2.08	0.67
1:A:195:ASP:HB2	1:A:201:LEU:N	2.08	0.67
1:A:290:PHE:HZ	1:A:296:TYR:OH	1.77	0.67
1:A:423:THR:HB	2:A:810:NAG:C8	2.24	0.67
1:A:403:ASN:HB2	3:A:902:NDG:N2	2.10	0.67
1:B:224:LYS:HE3	1:B:316:THR:O	1.95	0.67
1:B:187:TYR:HA	2:B:801:NAG:C8	2.25	0.67
1:A:224:LYS:HE3	1:A:316:THR:O	1.95	0.67
1:B:221:PHE:CE1	1:B:315:SER:O	2.45	0.67
1:B:403:ASN:HB2	3:B:902:NDG:N2	2.10	0.67
1:A:187:TYR:HA	2:A:801:NAG:C8	2.25	0.67
1:A:396:ARG:HD3	1:A:431:LEU:O	1.94	0.67
1:A:366:LYS:HG3	1:A:367:LEU:HG	1.77	0.66
1:B:423:THR:HB	2:B:810:NAG:C8	2.24	0.66
1:A:222:ASP:CG	1:A:222:ASP:O	2.32	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ARG:HD2	1:A:392:GLY:H	1.60	0.66
1:A:396:ARG:NH2	1:A:464:ILE:CB	2.58	0.66
1:B:482:THR:HG21	1:B:500:GLN:H	1.58	0.66
1:A:440:PRO:HA	1:A:458:THR:O	1.94	0.66
3:B:902:NDG:O7	3:B:902:NDG:H3	1.95	0.66
1:A:396:ARG:HE	1:A:432:ASP:CB	2.07	0.66
1:B:282:LEU:HD23	1:B:283:THR:H	1.58	0.66
1:B:373:ASN:ND2	1:B:374:ASP:N	2.43	0.66
1:B:464:ILE:O	1:B:467:ASN:HB2	1.96	0.66
1:A:320:THR:HG21	2:A:807:NAG:H2	1.76	0.66
1:A:88:VAL:HA	1:B:92:MET:HG2	1.76	0.66
1:B:137:ASP:OD2	1:B:139:ILE:HG22	1.94	0.66
1:B:482:THR:OG1	1:B:500:GLN:CG	2.44	0.66
1:B:440:PRO:HD2	1:B:522:LEU:CD1	2.26	0.66
1:A:401:VAL:HG13	1:A:405:THR:O	1.95	0.66
1:B:347:ARG:HD2	1:B:392:GLY:H	1.60	0.66
1:A:32:ASN:CG	1:A:33:LYS:H	1.98	0.66
1:A:373:ASN:ND2	1:A:374:ASP:N	2.43	0.66
1:A:446:THR:CG2	1:A:537:ILE:O	2.44	0.66
1:B:32:ASN:CG	1:B:33:LYS:H	1.98	0.66
1:B:366:LYS:HG3	1:B:367:LEU:HG	1.77	0.66
1:A:82:SER:OG	1:B:91:PRO:C	2.33	0.66
1:A:482:THR:OG1	1:A:500:GLN:CG	2.44	0.66
1:B:320:THR:HG21	2:B:807:NAG:H2	1.76	0.66
1:A:483:TRP:CZ2	1:A:507:TYR:HE1	2.09	0.66
1:A:488:ASP:HB2	1:A:493:SER:OG	1.97	0.65
2:A:805:NAG:C6	2:A:806:NAG:C7	2.74	0.65
1:B:524:VAL:HG21	2:B:904:NAG:H81	1.77	0.65
1:A:524:VAL:HG21	2:A:904:NAG:H81	1.77	0.65
1:B:405:THR:OG1	1:B:406:TYR:N	2.22	0.65
1:B:440:PRO:HD3	1:B:522:LEU:HD12	1.78	0.65
1:A:28:LYS:NZ	1:B:4:ILE:N	2.38	0.65
1:B:341:VAL:HG21	1:B:345:LEU:HD12	1.79	0.65
1:A:32:ASN:ND2	1:A:83:GLU:N	2.44	0.65
1:A:327:ASN:HA	1:A:360:ASP:OD2	1.97	0.65
1:A:464:ILE:O	1:A:467:ASN:HB2	1.96	0.65
1:B:195:ASP:HB2	1:B:201:LEU:N	2.08	0.65
2:B:809:NAG:C6	2:B:810:NAG:H62	2.26	0.65
1:B:474:SER:HB2	1:B:512:LEU:CG	2.15	0.65
1:B:482:THR:HG21	1:B:499:THR:CA	2.27	0.65
2:A:809:NAG:C6	2:A:810:NAG:H62	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ILE:O	1:A:364:ILE:HD12	1.97	0.64
1:B:524:VAL:HG23	2:B:904:NAG:H81	1.78	0.64
1:A:524:VAL:HG23	2:A:904:NAG:H81	1.78	0.64
1:B:364:ILE:HD12	1:B:364:ILE:O	1.98	0.64
1:B:403:ASN:HB2	3:B:902:NDG:H8C1	1.78	0.64
1:A:440:PRO:HD2	1:A:522:LEU:CD1	2.26	0.64
1:A:469:TYR:CD2	1:A:470:PRO:CD	2.81	0.64
1:B:232:GLU:HG3	1:B:290:PHE:H	1.61	0.64
1:B:446:THR:CG2	1:B:537:ILE:O	2.44	0.64
1:A:333:VAL:HB	1:A:334:PRO:CD	2.24	0.64
1:A:375:PRO:HB3	1:A:400:TYR:CD2	2.33	0.64
1:B:504:LYS:NZ	1:B:531:SER:OG	2.31	0.64
2:B:904:NAG:O7	2:B:904:NAG:C3	2.45	0.64
1:A:212:THR:HG22	1:A:213:ASP:H	1.62	0.64
1:B:347:ARG:HG3	1:B:392:GLY:H	1.62	0.64
1:B:406:TYR:CE1	2:B:808:NAG:H83	2.32	0.64
1:B:409:ILE:HG12	1:B:425:THR:HG23	1.80	0.64
1:A:346:SER:OG	1:A:349:GLU:HG3	1.97	0.64
1:B:488:ASP:HB2	1:B:493:SER:OG	1.97	0.64
1:B:227:THR:CG2	2:B:807:NAG:C7	2.76	0.64
1:A:486:GLU:O	1:A:494:MET:CA	2.46	0.64
1:B:32:ASN:ND2	1:B:83:GLU:N	2.44	0.64
1:A:486:GLU:O	1:A:495:LEU:N	2.31	0.64
1:A:406:TYR:CE1	2:A:808:NAG:H83	2.32	0.64
1:A:403:ASN:HB2	3:A:902:NDG:H8C1	1.78	0.64
1:A:232:GLU:HG3	1:A:290:PHE:H	1.61	0.63
1:A:419:VAL:HG13	2:A:809:NAG:O7	1.98	0.63
1:B:364:ILE:CD1	1:B:364:ILE:O	2.46	0.63
1:B:371:ILE:HG22	1:B:372:GLY:N	2.14	0.63
1:A:482:THR:HG22	1:A:499:THR:N	2.13	0.63
1:A:154:ASP:O	2:A:801:NAG:H82	1.98	0.63
1:B:346:SER:OG	1:B:349:GLU:HG3	1.97	0.63
1:A:347:ARG:HG3	1:A:392:GLY:H	1.62	0.63
1:A:518:ASN:O	1:A:520:PRO:CD	2.46	0.63
1:B:22:VAL:HG22	1:B:23:GLN:N	2.14	0.63
1:B:486:GLU:O	1:B:494:MET:CA	2.46	0.63
1:A:446:THR:CG2	1:A:539:CYS:SG	2.86	0.63
1:A:341:VAL:HG21	1:A:345:LEU:HD12	1.79	0.63
1:B:154:ASP:O	2:B:801:NAG:H82	1.98	0.63
1:B:419:VAL:HG13	2:B:809:NAG:O7	1.98	0.63
1:A:127:VAL:HG22	1:A:128:MET:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLU:HB3	1:A:433:VAL:CG2	2.28	0.63
1:A:482:THR:HG21	1:A:499:THR:CA	2.27	0.63
1:B:212:THR:HG22	1:B:213:ASP:H	1.62	0.63
1:B:327:ASN:HA	1:B:360:ASP:OD2	1.97	0.63
1:A:142:LEU:HB3	1:A:196:LEU:HA	1.81	0.63
1:B:375:PRO:HB3	1:B:400:TYR:CD2	2.33	0.63
1:B:446:THR:CG2	1:B:539:CYS:SG	2.86	0.63
1:B:154:ASP:CA	2:B:801:NAG:H82	2.29	0.63
1:B:403:ASN:CB	3:B:902:NDG:C7	2.76	0.63
1:A:364:ILE:O	1:A:364:ILE:CD1	2.46	0.63
1:A:87:PRO:CD	1:B:89:GLU:HB2	2.22	0.63
1:B:524:VAL:HG23	2:B:904:NAG:C8	2.29	0.63
1:A:154:ASP:CA	2:A:801:NAG:H82	2.29	0.62
1:A:504:LYS:NZ	1:A:531:SER:OG	2.31	0.62
2:A:904:NAG:O7	2:A:904:NAG:C3	2.45	0.62
1:B:142:LEU:HB3	1:B:196:LEU:HA	1.80	0.62
1:B:469:TYR:CD2	1:B:470:PRO:CD	2.81	0.62
1:A:22:VAL:HG22	1:A:23:GLN:N	2.14	0.62
1:B:482:THR:HG22	1:B:499:THR:N	2.13	0.62
1:A:371:ILE:HG22	1:A:372:GLY:N	2.14	0.62
1:A:524:VAL:HG23	2:A:904:NAG:C8	2.29	0.62
1:A:31:PHE:CG	1:B:93:GLU:OE2	2.52	0.62
1:A:374:ASP:O	1:A:375:PRO:O	2.17	0.62
1:B:343:GLU:HB3	1:B:433:VAL:CG2	2.28	0.62
1:B:368:SER:HG	1:B:370:PHE:HE1	1.47	0.62
1:A:409:ILE:HG12	1:A:425:THR:HG23	1.80	0.62
1:A:440:PRO:HD3	1:A:522:LEU:HD12	1.78	0.62
1:A:411:LEU:HD22	1:A:421:THR:HG23	1.81	0.62
1:B:147:SER:OG	1:B:167:ARG:HG3	1.99	0.62
1:B:265:GLU:HB3	1:B:268:PHE:CE2	2.31	0.62
1:B:517:GLN:C	1:B:519:ASN:N	2.47	0.62
1:B:222:ASP:O	1:B:222:ASP:CG	2.32	0.62
1:B:486:GLU:O	1:B:495:LEU:N	2.32	0.62
1:B:508:SER:HB3	1:B:526:ASN:OD1	2.00	0.62
1:A:508:SER:HB3	1:A:526:ASN:OD1	2.00	0.62
1:A:227:THR:CG2	2:A:807:NAG:C7	2.76	0.62
1:B:518:ASN:O	1:B:520:PRO:CD	2.46	0.62
1:A:524:VAL:CG2	2:A:904:NAG:C8	2.78	0.61
1:B:411:LEU:HD22	1:B:421:THR:HG23	1.81	0.61
1:B:449:ASP:H	1:B:532:CYS:CB	2.12	0.61
1:A:221:PHE:CE1	1:A:315:SER:O	2.45	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:THR:HG22	1:B:213:ASP:N	2.15	0.61
1:A:181:ARG:NE	1:A:213:ASP:OD1	2.34	0.61
1:A:403:ASN:O	1:A:405:THR:N	2.33	0.61
1:B:181:ARG:NE	1:B:213:ASP:OD1	2.34	0.61
1:B:524:VAL:CG2	2:B:904:NAG:C8	2.78	0.61
1:B:379:LEU:HD23	1:B:379:LEU:H	1.66	0.61
1:B:68:ARG:HD3	1:B:100:ASP:HA	1.82	0.61
1:B:127:VAL:HG22	1:B:128:MET:N	2.14	0.61
1:B:469:TYR:CE1	1:B:470:PRO:HD2	2.34	0.61
1:A:89:GLU:CD	1:B:3:VAL:HG13	2.20	0.61
1:B:374:ASP:O	1:B:375:PRO:O	2.17	0.61
1:A:469:TYR:CE1	1:A:470:PRO:HD2	2.34	0.61
1:B:154:ASP:O	1:B:155:PRO:C	2.36	0.61
1:B:475:LEU:O	1:B:479:SER:HB3	2.01	0.61
1:A:415:ASP:OD1	1:A:416:GLY:N	2.27	0.61
2:B:805:NAG:C6	2:B:806:NAG:C7	2.74	0.61
1:A:265:GLU:HB3	1:A:268:PHE:CE2	2.31	0.60
1:A:379:LEU:H	1:A:379:LEU:HD23	1.66	0.60
1:B:403:ASN:O	1:B:405:THR:N	2.33	0.60
1:A:371:ILE:CG2	1:A:372:GLY:H	2.13	0.60
1:A:68:ARG:HD3	1:A:100:ASP:HA	1.82	0.60
1:B:371:ILE:CG2	1:B:372:GLY:H	2.13	0.60
1:A:403:ASN:CB	3:A:902:NDG:C7	2.76	0.60
1:B:239:VAL:HG13	1:B:240:GLN:H	1.67	0.60
1:B:396:ARG:NH2	1:B:464:ILE:HG21	2.17	0.60
1:B:415:ASP:OD1	1:B:416:GLY:N	2.27	0.60
1:A:232:GLU:CG	1:A:290:PHE:N	2.64	0.60
1:A:212:THR:HG22	1:A:213:ASP:N	2.15	0.60
1:A:336:VAL:HB	1:A:426:LEU:HD23	1.84	0.60
1:A:154:ASP:O	1:A:155:PRO:C	2.36	0.60
1:A:475:LEU:O	1:A:479:SER:HB3	2.01	0.60
1:B:116:SER:HA	1:B:210:GLN:O	2.02	0.60
1:A:514:SER:HA	1:A:517:GLN:O	2.02	0.60
1:A:155:PRO:C	1:A:157:GLU:N	2.56	0.59
1:A:116:SER:HA	1:A:210:GLN:O	2.02	0.59
1:B:447:MET:HB2	1:B:529:VAL:HG22	1.84	0.59
1:B:189:LEU:N	1:B:189:LEU:HD23	2.17	0.59
1:A:189:LEU:HD23	1:A:189:LEU:N	2.17	0.59
1:A:146:LEU:HA	1:A:194:THR:O	2.02	0.59
1:A:49:GLY:O	1:A:63:THR:HG21	2.02	0.59
1:B:232:GLU:CG	1:B:290:PHE:N	2.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:VAL:HG13	1:A:240:GLN:H	1.67	0.59
1:B:367:LEU:CB	1:B:413:THR:O	2.51	0.59
1:B:221:PHE:HA	1:B:244:VAL:HG12	1.85	0.59
1:B:268:PHE:HA	1:B:285:ALA:HB3	1.85	0.59
1:B:38:ILE:HG22	1:B:53:ILE:HG22	1.85	0.59
1:A:363:GLN:O	1:A:364:ILE:HG22	2.03	0.59
1:A:268:PHE:HA	1:A:285:ALA:HB3	1.85	0.59
1:A:286:LYS:O	1:A:287:GLY:O	2.21	0.59
1:A:38:ILE:HG22	1:A:53:ILE:HG22	1.85	0.59
1:A:154:ASP:CB	2:A:801:NAG:HN2	2.16	0.59
1:B:232:GLU:HG2	1:B:289:ASP:CA	2.33	0.59
1:B:299:GLN:C	1:B:300:ILE:HD12	2.24	0.59
1:A:473:VAL:HA	1:A:513:LEU:HD23	1.85	0.58
1:B:514:SER:HA	1:B:517:GLN:O	2.02	0.58
1:B:473:VAL:HA	1:B:513:LEU:HD23	1.85	0.58
1:A:335:ALA:HB1	3:A:811:NDG:C6	2.33	0.58
1:B:195:ASP:CB	1:B:200:GLY:HA3	2.33	0.58
1:B:309:SER:O	1:B:310:VAL:HG23	2.03	0.58
1:B:443:ARG:HA	1:B:525:VAL:HG13	1.85	0.58
1:A:154:ASP:CB	1:A:155:PRO:CD	2.82	0.58
1:A:367:LEU:CB	1:A:413:THR:O	2.51	0.58
1:A:508:SER:HA	1:A:526:ASN:HA	1.84	0.58
1:B:146:LEU:HA	1:B:194:THR:O	2.02	0.58
1:A:537:ILE:HG12	1:A:538:LYS:N	2.19	0.58
1:B:363:GLN:O	1:B:364:ILE:HG22	2.03	0.58
1:B:336:VAL:HB	1:B:426:LEU:HD23	1.84	0.58
1:A:235:ILE:HG12	1:A:287:GLY:HA2	1.82	0.58
1:A:299:GLN:C	1:A:300:ILE:HD12	2.24	0.58
1:A:443:ARG:HA	1:A:525:VAL:HG13	1.85	0.58
1:B:443:ARG:HH11	1:B:443:ARG:HG3	1.67	0.58
1:A:221:PHE:HA	1:A:244:VAL:HG12	1.85	0.58
1:A:232:GLU:HG2	1:A:289:ASP:CA	2.33	0.58
1:B:332:PHE:CD2	1:B:424:GLY:HA3	2.39	0.58
1:B:154:ASP:CB	1:B:155:PRO:CD	2.82	0.58
1:B:406:TYR:HB3	1:B:428:LEU:CD2	2.33	0.58
1:B:42:GLY:HA2	1:B:47:PRO:O	2.04	0.58
1:B:49:GLY:O	1:B:63:THR:HG21	2.02	0.58
1:B:508:SER:HA	1:B:526:ASN:HA	1.84	0.58
1:A:309:SER:O	1:A:310:VAL:HG23	2.03	0.58
1:A:406:TYR:HB3	1:A:428:LEU:CD2	2.33	0.58
1:A:447:MET:HB2	1:A:529:VAL:HG22	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:THR:CG2	2:A:807:NAG:C2	2.76	0.57
1:B:450:GLN:HB2	1:B:533:GLU:CA	2.26	0.57
1:A:332:PHE:CD2	1:A:424:GLY:HA3	2.39	0.57
1:B:286:LYS:O	1:B:287:GLY:O	2.21	0.57
1:A:330:PRO:HD3	1:A:414:ASP:HB2	1.86	0.57
1:A:443:ARG:HG3	1:A:443:ARG:HH11	1.67	0.57
1:A:505:GLY:HA2	1:A:529:VAL:H	1.69	0.57
1:B:226:TYR:CE2	1:B:242:LEU:HD23	2.39	0.57
1:A:222:ASP:N	1:A:243:SER:O	2.38	0.57
1:A:42:GLY:HA2	1:A:47:PRO:O	2.04	0.57
1:B:330:PRO:HD3	1:B:414:ASP:HB2	1.86	0.57
1:B:537:ILE:HG12	1:B:538:LYS:N	2.19	0.57
1:A:68:ARG:HG3	1:A:69:GLU:N	2.19	0.57
1:A:240:GLN:HG3	1:A:241:ARG:N	2.19	0.57
1:B:505:GLY:HA2	1:B:529:VAL:H	1.70	0.57
1:A:517:GLN:C	1:A:519:ASN:N	2.47	0.57
1:A:195:ASP:CB	1:A:200:GLY:HA3	2.33	0.57
1:A:189:LEU:HD21	1:A:209:ILE:HD12	1.87	0.57
1:A:369:TYR:HD1	1:A:383:LYS:O	1.88	0.57
1:B:222:ASP:N	1:B:243:SER:O	2.38	0.57
1:B:240:GLN:HG3	1:B:241:ARG:N	2.19	0.56
1:B:296:TYR:HB2	1:B:321:VAL:HB	1.86	0.56
1:B:336:VAL:HG12	1:B:338:ARG:HB2	1.87	0.56
1:A:296:TYR:HB2	1:A:321:VAL:HB	1.86	0.56
1:A:449:ASP:H	1:A:532:CYS:CB	2.12	0.56
1:A:226:TYR:CE2	1:A:242:LEU:HD23	2.39	0.56
1:B:155:PRO:C	1:B:157:GLU:N	2.56	0.56
1:B:32:ASN:CG	1:B:33:LYS:N	2.59	0.56
1:B:378:TRP:O	1:B:391:ASN:HB2	2.06	0.56
1:A:108:PHE:CE1	1:A:203:VAL:HG23	2.40	0.56
1:A:396:ARG:NH2	1:A:464:ILE:HG21	2.17	0.56
1:B:394:LEU:CD1	1:B:394:LEU:N	2.69	0.56
1:A:336:VAL:HG12	1:A:338:ARG:HB2	1.87	0.56
1:A:155:PRO:N	2:A:801:NAG:H82	2.20	0.56
1:B:108:PHE:CE1	1:B:203:VAL:HG23	2.40	0.56
1:B:118:ARG:HA	1:B:212:THR:HB	1.87	0.56
1:B:335:ALA:HB1	3:B:811:NDG:C6	2.33	0.56
1:B:154:ASP:CB	2:B:801:NAG:HN2	2.16	0.56
1:B:32:ASN:HD22	1:B:83:GLU:H	1.51	0.56
1:B:189:LEU:HD21	1:B:209:ILE:HD12	1.87	0.56
1:B:393:ASN:C	1:B:394:LEU:HD12	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:TYR:O	1:B:260:LYS:HB3	2.05	0.56
1:B:333:VAL:CG2	1:B:334:PRO:HD3	2.36	0.56
1:B:369:TYR:HD1	1:B:383:LYS:O	1.88	0.56
1:A:162:LEU:O	1:A:174:LEU:HD12	2.06	0.56
1:A:394:LEU:N	1:A:394:LEU:CD1	2.69	0.55
1:B:365:GLN:CG	1:B:365:GLN:O	2.54	0.55
1:B:155:PRO:N	2:B:801:NAG:H82	2.20	0.55
1:A:259:TYR:O	1:A:260:LYS:HB3	2.05	0.55
1:B:68:ARG:HG3	1:B:69:GLU:N	2.19	0.55
1:B:339:VAL:HG21	1:B:351:ILE:CG2	2.37	0.55
1:A:118:ARG:HA	1:A:212:THR:HB	1.87	0.55
1:A:393:ASN:C	1:A:394:LEU:HD12	2.25	0.55
1:A:459:ILE:HG21	1:A:471:TYR:CE2	2.42	0.55
1:A:32:ASN:HD22	1:A:83:GLU:H	1.51	0.55
1:B:272:THR:CG2	1:B:273:THR:H	2.19	0.55
1:A:339:VAL:HG21	1:A:351:ILE:CG2	2.36	0.55
1:A:406:TYR:HB3	1:A:428:LEU:HD21	1.87	0.55
1:B:406:TYR:HB3	1:B:428:LEU:HD21	1.87	0.55
1:A:154:ASP:CG	1:A:155:PRO:CD	2.75	0.55
1:A:241:ARG:NE	1:A:281:ILE:HD12	2.22	0.55
1:A:32:ASN:CG	1:A:33:LYS:N	2.59	0.55
1:A:439:VAL:HG13	1:A:522:LEU:HD11	1.88	0.55
1:B:278:ASN:HD22	1:B:278:ASN:N	2.05	0.55
1:A:272:THR:CG2	1:A:273:THR:H	2.19	0.55
1:A:378:TRP:O	1:A:391:ASN:HB2	2.06	0.55
1:B:28:LYS:HB3	1:B:88:VAL:HG11	1.89	0.55
1:B:482:THR:HG21	1:B:499:THR:C	2.27	0.55
1:A:155:PRO:HG2	2:A:801:NAG:O7	2.07	0.55
1:A:466:PRO:O	1:A:468:THR:N	2.40	0.55
1:B:162:LEU:O	1:B:174:LEU:HD12	2.06	0.55
1:B:117:VAL:O	1:B:211:ILE:HA	2.07	0.55
1:A:169:THR:OG1	1:A:171:VAL:HG23	2.07	0.55
1:B:226:TYR:O	1:B:227:THR:CG2	2.55	0.55
1:B:330:PRO:HB3	1:B:358:ASP:HB2	1.89	0.55
1:B:466:PRO:O	1:B:468:THR:N	2.40	0.55
1:B:75:VAL:O	1:B:76:LEU:HD23	2.07	0.55
1:A:333:VAL:CG2	1:A:334:PRO:HD3	2.36	0.54
1:B:419:VAL:CG1	1:B:420:GLY:N	2.70	0.54
1:A:226:TYR:HB2	1:A:319:VAL:HG22	1.90	0.54
1:B:438:PRO:HB2	1:B:513:LEU:HD12	1.89	0.54
1:A:226:TYR:O	1:A:227:THR:CG2	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LEU:C	1:A:367:LEU:HD12	2.28	0.54
1:A:419:VAL:CG1	1:A:420:GLY:N	2.70	0.54
1:B:403:ASN:HB2	3:B:902:NDG:H8C2	1.87	0.54
1:B:363:GLN:C	1:B:364:ILE:CG2	2.75	0.54
1:A:84:ASN:ND2	1:B:77:SER:OG	2.41	0.54
1:B:155:PRO:HG2	2:B:801:NAG:O7	2.07	0.54
1:A:482:THR:HG21	1:A:499:THR:C	2.27	0.54
1:A:75:VAL:O	1:A:76:LEU:HD23	2.08	0.54
1:B:235:ILE:HG12	1:B:287:GLY:HA2	1.82	0.54
1:B:154:ASP:CG	1:B:155:PRO:CD	2.75	0.54
1:B:367:LEU:HD12	1:B:367:LEU:C	2.28	0.54
1:A:363:GLN:C	1:A:364:ILE:CG2	2.76	0.54
1:A:438:PRO:HB2	1:A:513:LEU:HD12	1.89	0.54
1:A:371:ILE:HG23	1:A:372:GLY:H	1.73	0.54
1:B:439:VAL:HG13	1:B:522:LEU:HD11	1.88	0.54
1:B:432:ASP:CG	1:B:464:ILE:CG2	2.74	0.54
1:A:82:SER:OG	1:B:91:PRO:N	2.40	0.54
1:A:154:ASP:C	2:A:801:NAG:C8	2.62	0.54
1:A:22:VAL:HG22	1:A:23:GLN:H	1.73	0.54
1:A:318:THR:CG2	2:A:806:NAG:H5	2.34	0.54
1:B:332:PHE:HD2	1:B:424:GLY:HA3	1.73	0.54
1:B:490:LYS:O	1:B:490:LYS:HG2	2.08	0.54
1:A:117:VAL:O	1:A:211:ILE:HA	2.07	0.54
1:B:459:ILE:HG21	1:B:471:TYR:CE2	2.42	0.54
1:B:443:ARG:HG3	1:B:443:ARG:NH1	2.23	0.53
1:A:84:ASN:ND2	1:B:79:HIS:CE1	2.76	0.53
1:A:28:LYS:HB3	1:A:88:VAL:HG11	1.89	0.53
1:A:373:ASN:HB3	1:A:409:ILE:H	1.74	0.53
1:B:450:GLN:CB	1:B:532:CYS:O	2.56	0.53
1:A:330:PRO:HB3	1:A:358:ASP:HB2	1.89	0.53
1:B:249:MET:O	1:B:252:THR:HB	2.08	0.53
1:B:268:PHE:N	1:B:268:PHE:CD2	2.75	0.53
1:B:403:ASN:C	1:B:405:THR:H	2.12	0.53
1:B:458:THR:HG22	1:B:493:SER:HB3	1.90	0.53
1:B:252:THR:HG23	1:B:253:PRO:HD2	1.90	0.53
1:B:276:GLU:CG	1:B:277:SER:N	2.71	0.53
1:A:369:TYR:O	1:A:383:LYS:HG2	2.09	0.53
1:A:450:GLN:CB	1:A:532:CYS:O	2.56	0.53
1:B:105:ARG:HG3	1:B:106:PRO:HD2	1.91	0.53
1:B:217:ASN:N	1:B:217:ASN:ND2	2.56	0.53
1:A:249:MET:O	1:A:252:THR:HB	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:LEU:CD2	1:A:523:THR:HB	2.26	0.53
1:A:533:GLU:OE2	1:A:533:GLU:HA	2.09	0.53
1:B:533:GLU:HA	1:B:533:GLU:OE2	2.09	0.53
1:A:347:ARG:HG3	1:A:391:ASN:HA	1.91	0.53
1:A:88:VAL:HA	1:B:92:MET:CG	2.39	0.53
1:B:312:LEU:O	3:B:804:NDG:C8	2.57	0.53
1:A:242:LEU:O	1:A:279:GLN:HB3	2.09	0.53
1:A:276:GLU:CG	1:A:277:SER:N	2.71	0.53
1:A:458:THR:HG22	1:A:493:SER:HB3	1.91	0.53
1:B:169:THR:OG1	1:B:171:VAL:HG23	2.07	0.53
1:B:22:VAL:HG22	1:B:23:GLN:H	1.73	0.53
1:B:450:GLN:CB	1:B:533:GLU:HA	2.29	0.53
1:B:318:THR:CG2	2:B:806:NAG:H5	2.34	0.53
1:A:105:ARG:HG3	1:A:106:PRO:HD2	1.91	0.53
1:A:367:LEU:HD13	1:A:412:VAL:HG23	1.91	0.53
1:A:512:LEU:HD11	1:A:519:ASN:HD21	1.74	0.53
1:A:84:ASN:CG	1:B:77:SER:HG	2.12	0.53
1:B:352:ILE:CG1	1:B:388:VAL:HB	2.33	0.53
1:B:367:LEU:HD13	1:B:412:VAL:HG23	1.91	0.53
1:B:482:THR:O	1:B:482:THR:HG22	2.09	0.53
1:B:512:LEU:HD11	1:B:519:ASN:HD21	1.74	0.53
1:B:242:LEU:O	1:B:279:GLN:HB3	2.09	0.52
1:B:226:TYR:HB2	1:B:319:VAL:HG22	1.89	0.52
1:B:426:LEU:HD13	1:B:426:LEU:O	2.10	0.52
1:A:217:ASN:ND2	1:A:217:ASN:N	2.56	0.52
1:A:268:PHE:C	1:A:285:ALA:HB3	2.30	0.52
1:A:523:THR:CG2	1:A:524:VAL:H	1.94	0.52
1:A:312:LEU:O	3:A:804:NDG:C8	2.57	0.52
1:A:194:THR:HG22	1:A:195:ASP:N	2.25	0.52
1:B:194:THR:HG22	1:B:195:ASP:N	2.25	0.52
1:B:268:PHE:C	1:B:285:ALA:HB3	2.30	0.52
1:B:347:ARG:HG3	1:B:391:ASN:HA	1.91	0.52
1:A:403:ASN:C	1:A:405:THR:H	2.12	0.52
1:A:82:SER:O	1:B:90:GLU:OE2	2.25	0.52
1:B:227:THR:CG2	2:B:807:NAG:H83	2.32	0.52
1:A:432:ASP:CG	1:A:464:ILE:CG2	2.74	0.52
1:B:373:ASN:HB3	1:B:409:ILE:H	1.74	0.52
1:A:252:THR:HG23	1:A:253:PRO:HD2	1.91	0.52
1:A:379:LEU:CD2	1:A:379:LEU:H	2.22	0.52
1:A:90:GLU:CB	1:B:2:TRP:CD1	2.92	0.52
1:B:369:TYR:O	1:B:383:LYS:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ARG:CZ	1:B:432:ASP:HB2	2.40	0.52
1:A:31:PHE:CD2	1:A:32:ASN:HB2	2.44	0.52
1:A:33:LYS:HB3	1:A:83:GLU:CG	2.40	0.52
1:A:332:PHE:HD2	1:A:424:GLY:HA3	1.73	0.52
1:A:450:GLN:HB2	1:A:533:GLU:CA	2.26	0.52
1:B:155:PRO:CD	2:B:801:NAG:H82	2.40	0.52
1:A:403:ASN:HB2	3:A:902:NDG:H8C2	1.87	0.51
1:B:221:PHE:HB3	1:B:223:PRO:O	2.10	0.51
1:B:31:PHE:CD2	1:B:32:ASN:HB2	2.44	0.51
1:A:458:THR:HA	1:A:493:SER:HA	1.93	0.51
1:B:371:ILE:HG23	1:B:372:GLY:H	1.73	0.51
1:B:482:THR:CG2	1:B:499:THR:CA	2.87	0.51
1:B:272:THR:CG2	2:B:803:NAG:HN2	2.23	0.51
1:B:8:LYS:N	1:B:8:LYS:CD	2.51	0.51
1:A:471:TYR:N	1:A:471:TYR:CD1	2.79	0.51
1:A:428:LEU:O	1:A:428:LEU:HD23	2.11	0.51
1:B:333:VAL:CB	1:B:334:PRO:CD	2.88	0.51
1:B:514:SER:HB3	1:B:517:GLN:O	2.10	0.51
1:A:426:LEU:HD13	1:A:426:LEU:O	2.10	0.51
1:A:482:THR:CG2	1:A:499:THR:CA	2.87	0.51
1:A:505:GLY:O	1:A:506:ASP:OD1	2.28	0.51
1:A:151:LEU:HD12	1:A:190:THR:O	2.11	0.51
1:A:336:VAL:O	1:A:426:LEU:HD22	2.10	0.51
1:A:514:SER:HB3	1:A:517:GLN:O	2.10	0.51
1:A:155:PRO:CD	2:A:801:NAG:H82	2.40	0.51
1:B:450:GLN:CG	1:B:533:GLU:OE2	2.58	0.51
1:B:471:TYR:CD1	1:B:471:TYR:N	2.79	0.51
1:B:505:GLY:O	1:B:506:ASP:OD1	2.28	0.51
1:B:522:LEU:CD2	1:B:523:THR:HB	2.26	0.51
2:B:809:NAG:H61	2:B:810:NAG:C6	2.39	0.51
1:A:365:GLN:CG	1:A:365:GLN:O	2.54	0.51
1:B:154:ASP:C	2:B:801:NAG:C8	2.62	0.51
1:A:272:THR:CG2	2:A:803:NAG:HN2	2.23	0.51
1:B:142:LEU:O	1:B:196:LEU:HD23	2.11	0.51
1:B:458:THR:HG22	1:B:493:SER:CB	2.41	0.51
1:A:142:LEU:O	1:A:196:LEU:HD23	2.11	0.51
1:A:297:VAL:CG2	2:A:807:NAG:H62	2.41	0.51
1:B:138:ASN:C	1:B:138:ASN:HD22	2.13	0.50
1:B:382:ASN:OD1	1:B:385:ASN:N	2.45	0.50
1:B:397:GLU:OE1	1:B:397:GLU:N	2.44	0.50
1:B:336:VAL:O	1:B:426:LEU:HD22	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ASN:C	1:A:138:ASN:HD22	2.13	0.50
1:A:221:PHE:HB3	1:A:223:PRO:O	2.10	0.50
1:A:347:ARG:HD2	1:A:392:GLY:N	2.25	0.50
1:A:496:LEU:HD21	1:A:509:ILE:CD1	2.38	0.50
1:A:449:ASP:CB	1:A:532:CYS:H	2.22	0.50
1:A:450:GLN:CG	1:A:533:GLU:OE2	2.58	0.50
1:B:154:ASP:O	2:B:801:NAG:C8	2.60	0.50
1:B:217:ASN:N	1:B:217:ASN:HD22	2.09	0.50
1:B:428:LEU:HD23	1:B:428:LEU:O	2.11	0.50
1:A:396:ARG:CZ	1:A:432:ASP:HB2	2.41	0.50
1:A:155:PRO:HG2	2:A:801:NAG:C7	2.42	0.50
1:B:261:ILE:HD11	1:B:264:ASN:HD22	1.77	0.50
1:A:154:ASP:O	2:A:801:NAG:C8	2.60	0.50
1:B:368:SER:OG	1:B:370:PHE:HE1	1.94	0.50
1:B:28:LYS:CD	1:B:88:VAL:HG12	2.38	0.50
1:A:234:GLU:HB2	1:A:235:ILE:HG22	1.93	0.50
1:A:278:ASN:N	1:A:278:ASN:HD22	2.05	0.50
1:B:347:ARG:HD2	1:B:392:GLY:N	2.25	0.50
1:A:457:LEU:HD23	1:A:494:MET:SD	2.52	0.50
1:A:449:ASP:CB	1:A:532:CYS:N	2.74	0.50
1:B:419:VAL:HG22	2:B:809:NAG:H81	1.93	0.50
1:B:423:THR:HB	2:B:810:NAG:H83	1.94	0.50
1:A:216:ASP:HB2	1:A:217:ASN:ND2	2.27	0.50
1:A:84:ASN:CB	1:B:79:HIS:CE1	2.62	0.50
1:B:151:LEU:HD12	1:B:190:THR:O	2.11	0.50
1:B:276:GLU:HG3	1:B:277:SER:N	2.25	0.50
1:B:338:ARG:HB3	1:B:339:VAL:HG22	1.92	0.50
1:B:457:LEU:HD23	1:B:494:MET:SD	2.52	0.50
1:B:297:VAL:CG2	2:B:807:NAG:H62	2.41	0.50
1:A:11:GLU:OE2	1:A:69:GLU:OE1	2.30	0.50
1:A:186:GLU:OE1	2:A:801:NAG:C6	2.59	0.50
1:A:458:THR:HG22	1:A:493:SER:CB	2.42	0.50
1:B:241:ARG:NE	1:B:281:ILE:HD12	2.22	0.50
1:B:363:GLN:C	1:B:364:ILE:HG23	2.32	0.50
1:B:432:ASP:CB	1:B:464:ILE:CG2	2.89	0.50
1:B:458:THR:HA	1:B:493:SER:HA	1.93	0.50
2:B:807:NAG:H3	2:B:807:NAG:O7	2.11	0.50
1:B:80:ALA:O	1:B:88:VAL:HG23	2.11	0.50
1:A:217:ASN:HD22	1:A:217:ASN:N	2.10	0.50
1:A:266:GLY:N	1:A:268:PHE:CE2	2.76	0.50
1:A:382:ASN:OD1	1:A:385:ASN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ARG:NH1	1:A:443:ARG:HG3	2.24	0.50
1:A:80:ALA:O	1:A:88:VAL:HG23	2.11	0.50
1:A:335:ALA:CB	3:A:811:NDG:C6	2.90	0.50
1:A:338:ARG:HB3	1:A:339:VAL:HG22	1.92	0.49
1:B:109:THR:HG22	1:B:110:GLN:HG3	1.94	0.49
1:B:155:PRO:HG2	2:B:801:NAG:C7	2.42	0.49
1:B:27:ASN:C	1:B:29:ASP:H	2.15	0.49
1:B:496:LEU:HD21	1:B:509:ILE:CD1	2.38	0.49
1:A:27:ASN:C	1:A:29:ASP:H	2.15	0.49
1:A:419:VAL:HG22	2:A:809:NAG:H81	1.94	0.49
1:B:151:LEU:H	1:B:151:LEU:HD12	1.78	0.49
1:A:155:PRO:O	1:A:157:GLU:N	2.43	0.49
1:A:432:ASP:CB	1:A:464:ILE:CG2	2.89	0.49
1:A:76:LEU:O	1:A:94:ILE:N	2.44	0.49
1:B:252:THR:CG2	1:B:253:PRO:HD2	2.43	0.49
1:B:273:THR:H	2:B:803:NAG:HN2	1.61	0.49
1:A:352:ILE:HG13	1:A:388:VAL:CB	2.33	0.49
1:A:273:THR:H	2:A:803:NAG:HN2	1.60	0.49
1:A:82:SER:H	1:B:90:GLU:C	2.15	0.49
1:B:216:ASP:HB2	1:B:217:ASN:ND2	2.27	0.49
1:B:402:LYS:C	1:B:403:ASN:O	2.46	0.49
1:B:76:LEU:O	1:B:94:ILE:N	2.44	0.49
1:A:261:ILE:HD11	1:A:264:ASN:HD22	1.77	0.49
1:A:290:PHE:CE2	1:A:293:ARG:CB	2.92	0.49
1:A:327:ASN:OD1	1:A:360:ASP:OD1	2.30	0.49
1:A:363:GLN:C	1:A:364:ILE:HG23	2.32	0.49
1:A:368:SER:OG	1:A:370:PHE:HE1	1.94	0.49
1:A:512:LEU:HD11	1:A:519:ASN:ND2	2.28	0.49
1:B:234:GLU:HB2	1:B:235:ILE:HG22	1.93	0.49
1:A:282:LEU:CD2	1:A:283:THR:N	2.76	0.49
1:A:482:THR:O	1:A:482:THR:HG22	2.09	0.49
1:A:352:ILE:CG1	1:A:388:VAL:HB	2.33	0.49
1:A:451:ASN:O	1:A:534:GLY:CA	2.60	0.49
2:A:807:NAG:H3	2:A:807:NAG:O7	2.11	0.49
1:B:281:ILE:O	1:B:281:ILE:HG23	2.13	0.49
1:B:282:LEU:CD2	1:B:283:THR:N	2.76	0.49
1:B:373:ASN:ND2	1:B:374:ASP:OD1	2.45	0.49
1:B:320:THR:CG2	2:B:807:NAG:C2	2.76	0.49
1:A:268:PHE:CD2	1:A:268:PHE:N	2.75	0.49
1:A:68:ARG:HD3	1:A:100:ASP:CA	2.43	0.49
1:B:109:THR:HG22	1:B:110:GLN:CG	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:GLN:HA	1:B:203:VAL:O	2.13	0.49
2:B:809:NAG:H62	2:B:810:NAG:O6	2.13	0.49
1:A:151:LEU:HD12	1:A:151:LEU:H	1.78	0.49
1:A:226:TYR:C	1:A:227:THR:HG23	2.33	0.49
1:B:11:GLU:OE2	1:B:69:GLU:OE1	2.30	0.49
1:B:33:LYS:HB3	1:B:83:GLU:CG	2.40	0.49
1:B:327:ASN:OD1	1:B:360:ASP:OD1	2.30	0.49
1:B:335:ALA:CB	3:B:811:NDG:C6	2.90	0.49
1:A:310:VAL:HG12	1:A:312:LEU:HG	1.95	0.49
1:A:336:VAL:CG1	1:A:338:ARG:HB2	2.43	0.49
1:A:397:GLU:OE1	1:A:397:GLU:N	2.45	0.49
1:A:423:THR:HB	2:A:810:NAG:H83	1.94	0.49
1:A:432:ASP:CB	1:A:464:ILE:HG21	2.43	0.49
1:B:310:VAL:HG12	1:B:312:LEU:HG	1.95	0.49
1:A:365:GLN:HA	1:A:416:GLY:HA3	1.95	0.48
2:A:809:NAG:H62	2:A:810:NAG:O6	2.13	0.48
1:A:8:LYS:CD	1:A:8:LYS:N	2.51	0.48
1:B:154:ASP:CG	1:B:155:PRO:HD2	2.33	0.48
1:B:186:GLU:OE1	2:B:801:NAG:C6	2.59	0.48
1:B:512:LEU:HD11	1:B:519:ASN:ND2	2.28	0.48
1:A:367:LEU:HD13	1:A:412:VAL:CG2	2.43	0.48
1:A:41:GLN:HA	1:A:45:ASN:HB2	1.95	0.48
1:B:266:GLY:N	1:B:268:PHE:CE2	2.76	0.48
1:B:41:GLN:HA	1:B:45:ASN:HB2	1.96	0.48
1:A:154:ASP:CG	1:A:155:PRO:HD2	2.33	0.48
1:A:224:LYS:CE	2:A:806:NAG:C8	2.91	0.48
1:A:224:LYS:HE3	2:A:806:NAG:H82	1.95	0.48
1:A:89:GLU:OE2	1:B:3:VAL:CG1	2.55	0.48
1:B:224:LYS:CE	2:B:806:NAG:C8	2.91	0.48
1:B:336:VAL:CG1	1:B:338:ARG:HB2	2.43	0.48
1:B:432:ASP:CB	1:B:464:ILE:HG21	2.43	0.48
1:A:250:PRO:O	1:A:255:TRP:CE3	2.66	0.48
1:A:373:ASN:ND2	1:A:374:ASP:OD1	2.45	0.48
1:B:151:LEU:O	1:B:152:LYS:HB2	2.13	0.48
1:A:109:THR:HG22	1:A:110:GLN:CG	2.42	0.48
1:A:109:THR:HG22	1:A:110:GLN:HG3	1.94	0.48
1:A:281:ILE:O	1:A:281:ILE:HG23	2.13	0.48
1:B:119:GLU:OE2	1:B:216:ASP:OD1	2.32	0.48
1:B:155:PRO:O	1:B:157:GLU:N	2.43	0.48
1:B:352:ILE:HG13	1:B:388:VAL:CB	2.33	0.48
1:B:367:LEU:HD13	1:B:412:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLN:HA	1:A:203:VAL:O	2.13	0.48
1:A:252:THR:CG2	1:A:253:PRO:HD2	2.43	0.48
1:A:333:VAL:CB	1:A:334:PRO:CD	2.88	0.48
1:B:150:ILE:HD11	1:B:165:ILE:HB	1.96	0.48
1:B:367:LEU:HB2	1:B:413:THR:O	2.12	0.48
1:B:67:ASP:OD2	1:B:69:GLU:HB2	2.13	0.48
2:B:812:NAG:O7	2:B:812:NAG:C1	2.60	0.48
1:A:151:LEU:O	1:A:152:LYS:HB2	2.13	0.48
1:B:226:TYR:C	1:B:227:THR:HG23	2.33	0.48
1:A:367:LEU:HB2	1:A:413:THR:O	2.12	0.48
1:B:250:PRO:O	1:B:255:TRP:CE3	2.66	0.48
1:B:225:THR:HA	1:B:318:THR:O	2.14	0.48
1:B:365:GLN:HA	1:B:416:GLY:HA3	1.95	0.48
1:A:366:LYS:HG2	1:A:367:LEU:H	1.75	0.47
2:A:809:NAG:H61	2:A:810:NAG:C6	2.39	0.47
1:B:68:ARG:HD3	1:B:100:ASP:CA	2.43	0.47
1:A:119:GLU:OE2	1:A:216:ASP:OD1	2.32	0.47
1:A:246:ASP:C	1:A:247:LEU:HD12	2.35	0.47
1:A:67:ASP:OD2	1:A:69:GLU:HB2	2.13	0.47
1:B:224:LYS:HE3	2:B:806:NAG:H82	1.95	0.47
1:B:418:SER:O	1:B:419:VAL:HG23	2.14	0.47
2:B:809:NAG:C6	2:B:810:NAG:C6	2.92	0.47
1:A:226:TYR:O	1:A:227:THR:HG23	2.15	0.47
1:A:448:CYS:SG	1:A:537:ILE:CG2	3.01	0.47
1:A:450:GLN:CB	1:A:533:GLU:HA	2.29	0.47
1:A:537:ILE:CG1	1:A:538:LYS:N	2.77	0.47
1:B:537:ILE:CG1	1:B:538:LYS:N	2.77	0.47
1:A:82:SER:C	1:B:90:GLU:HG3	2.21	0.47
1:A:514:SER:HG	1:A:519:ASN:HA	1.79	0.47
2:A:809:NAG:C6	2:A:810:NAG:C6	2.92	0.47
1:B:300:ILE:N	1:B:300:ILE:HD12	2.29	0.47
1:A:227:THR:CG2	2:A:807:NAG:H83	2.32	0.47
1:B:514:SER:CA	1:B:517:GLN:O	2.62	0.47
1:A:117:VAL:O	1:A:212:THR:N	2.46	0.47
1:B:268:PHE:CA	1:B:285:ALA:HB3	2.45	0.47
1:B:301:THR:CG2	1:B:316:THR:HG23	2.45	0.47
1:A:261:ILE:CD1	1:A:264:ASN:ND2	2.77	0.47
1:A:301:THR:CG2	1:A:316:THR:HG23	2.45	0.47
1:A:402:LYS:C	1:A:403:ASN:O	2.46	0.47
1:A:514:SER:CA	1:A:517:GLN:O	2.62	0.47
2:A:812:NAG:C1	2:A:812:NAG:O7	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ILE:CD1	1:B:264:ASN:ND2	2.77	0.47
1:A:300:ILE:HD12	1:A:300:ILE:N	2.29	0.47
1:A:225:THR:HA	1:A:318:THR:O	2.14	0.47
1:B:108:PHE:HE1	1:B:203:VAL:HG23	1.80	0.47
1:B:246:ASP:C	1:B:247:LEU:HD12	2.35	0.47
1:B:449:ASP:CB	1:B:532:CYS:N	2.74	0.47
1:A:108:PHE:HE1	1:A:203:VAL:HG23	1.80	0.47
1:A:150:ILE:HD11	1:A:165:ILE:HB	1.96	0.47
1:A:276:GLU:HG3	1:A:277:SER:N	2.25	0.47
1:A:23:GLN:HB2	1:A:59:TRP:CE3	2.50	0.47
1:A:268:PHE:CA	1:A:285:ALA:HB3	2.45	0.47
1:A:320:THR:CB	2:A:807:NAG:N2	2.78	0.47
1:B:310:VAL:HG12	1:B:311:PRO:O	2.15	0.47
1:B:36:TYR:O	1:B:55:TRP:HA	2.15	0.47
1:A:262:ARG:HG3	1:A:299:GLN:HB2	1.98	0.46
1:B:226:TYR:O	1:B:227:THR:HG23	2.15	0.46
1:B:379:LEU:CD2	1:B:379:LEU:H	2.22	0.46
1:A:310:VAL:HG12	1:A:311:PRO:O	2.15	0.46
1:B:272:THR:HG23	2:B:803:NAG:HN2	1.81	0.46
1:A:27:ASN:ND2	1:A:28:LYS:N	2.50	0.46
1:B:50:VAL:HB	1:B:51:PHE:CD1	2.50	0.46
1:B:270:ASN:OD1	1:B:271:ILE:N	2.49	0.46
1:B:371:ILE:HD12	1:B:371:ILE:HA	1.65	0.46
1:A:241:ARG:HE	1:A:281:ILE:CD1	2.24	0.46
1:A:374:ASP:OD1	1:A:374:ASP:N	2.49	0.46
1:A:418:SER:O	1:A:419:VAL:HG23	2.14	0.46
1:A:272:THR:HG23	2:A:803:NAG:HN2	1.81	0.46
1:B:290:PHE:CE2	1:B:293:ARG:CB	2.92	0.46
1:B:54:GLU:HB2	1:B:57:THR:OG1	2.16	0.46
1:B:227:THR:N	2:B:812:NAG:H2	2.31	0.46
1:A:194:THR:CG2	1:A:195:ASP:N	2.79	0.46
1:A:270:ASN:OD1	1:A:271:ILE:N	2.49	0.46
1:B:374:ASP:OD1	1:B:374:ASP:N	2.49	0.46
1:A:187:TYR:HE1	1:A:211:ILE:HD11	1.81	0.46
1:A:415:ASP:CG	1:A:416:GLY:H	2.16	0.46
1:A:50:VAL:HB	1:A:51:PHE:CD1	2.50	0.46
1:B:109:THR:CB	1:B:131:SER:HB2	2.46	0.46
1:B:23:GLN:HB2	1:B:59:TRP:CE3	2.50	0.46
1:B:363:GLN:O	1:B:364:ILE:CG2	2.63	0.46
1:B:371:ILE:HD13	1:B:381:VAL:HG11	1.95	0.46
1:B:415:ASP:CG	1:B:416:GLY:H	2.17	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:ILE:HD12	1:B:459:ILE:N	2.31	0.46
1:B:320:THR:CB	2:B:807:NAG:N2	2.78	0.46
1:A:373:ASN:CG	1:A:374:ASP:H	2.18	0.46
1:A:5:PRO:HA	1:A:6:PRO:HD3	1.86	0.46
1:B:271:ILE:HG23	1:B:271:ILE:O	2.15	0.46
1:A:506:ASP:OD1	1:A:506:ASP:N	2.49	0.46
1:A:54:GLU:HB2	1:A:57:THR:OG1	2.16	0.46
1:A:84:ASN:O	1:B:79:HIS:CE1	2.69	0.46
1:B:100:ASP:OD1	1:B:101:GLN:N	2.49	0.46
1:B:187:TYR:HE1	1:B:211:ILE:HD11	1.81	0.46
1:B:373:ASN:CG	1:B:374:ASP:H	2.18	0.46
1:A:461:ASP:HB3	1:A:468:THR:CG2	2.46	0.46
1:A:36:TYR:O	1:A:55:TRP:HA	2.15	0.46
1:B:227:THR:HG22	1:B:320:THR:HB	1.98	0.46
2:B:805:NAG:C5	2:B:806:NAG:H83	2.46	0.46
1:A:227:THR:HG22	1:A:320:THR:HB	1.98	0.45
1:A:227:THR:N	2:A:812:NAG:H2	2.31	0.45
1:B:194:THR:CG2	1:B:195:ASP:N	2.79	0.45
1:A:100:ASP:OD1	1:A:101:GLN:N	2.49	0.45
1:A:152:LYS:O	1:A:189:LEU:HA	2.17	0.45
1:A:363:GLN:O	1:A:364:ILE:CG2	2.64	0.45
1:A:473:VAL:CG2	1:A:487:LEU:HD21	2.47	0.45
1:A:511:VAL:N	1:A:523:THR:O	2.46	0.45
1:B:506:ASP:N	1:B:506:ASP:OD1	2.49	0.45
1:A:408:VAL:O	1:A:426:LEU:N	2.49	0.45
1:A:459:ILE:N	1:A:459:ILE:HD12	2.31	0.45
1:B:421:THR:HG21	2:B:809:NAG:H61	1.98	0.45
1:A:380:THR:CG2	1:A:381:VAL:N	2.79	0.45
1:B:252:THR:HA	1:B:253:PRO:HD3	1.81	0.45
1:A:162:LEU:HB2	1:A:163:PHE:CE1	2.52	0.45
1:B:261:ILE:HD11	1:B:264:ASN:ND2	2.32	0.45
1:B:380:THR:CG2	1:B:381:VAL:N	2.79	0.45
1:A:109:THR:CB	1:A:131:SER:HB2	2.46	0.45
1:A:155:PRO:CB	2:A:801:NAG:C8	2.94	0.45
1:B:381:VAL:HA	1:B:387:ILE:O	2.16	0.45
1:B:461:ASP:HB3	1:B:468:THR:CG2	2.46	0.45
1:B:469:TYR:CD2	1:B:470:PRO:N	2.85	0.45
1:A:271:ILE:O	1:A:271:ILE:HG23	2.15	0.45
1:A:380:THR:HG22	1:A:381:VAL:N	2.32	0.45
1:A:469:TYR:CD2	1:A:470:PRO:N	2.85	0.45
1:A:469:TYR:CE2	1:A:470:PRO:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:THR:HB	1:B:131:SER:HB2	1.99	0.45
1:B:286:LYS:C	1:B:287:GLY:O	2.55	0.45
1:B:408:VAL:O	1:B:426:LEU:N	2.49	0.45
1:A:336:VAL:HG11	1:A:338:ARG:HD2	1.99	0.45
2:A:805:NAG:C5	2:A:806:NAG:H83	2.46	0.45
1:B:272:THR:CG2	1:B:273:THR:N	2.76	0.45
1:B:426:LEU:HD13	1:B:426:LEU:C	2.37	0.45
1:B:469:TYR:CE2	1:B:470:PRO:HB2	2.52	0.45
1:B:482:THR:O	1:B:483:TRP:CD2	2.70	0.45
1:A:109:THR:HB	1:A:131:SER:HB2	1.99	0.45
1:A:312:LEU:O	3:A:804:NDG:H8C1	2.17	0.45
1:A:421:THR:HG21	2:A:809:NAG:H61	1.98	0.45
1:A:450:GLN:CB	1:A:533:GLU:OE2	2.64	0.45
1:B:339:VAL:HG11	1:B:351:ILE:HG23	1.98	0.45
1:B:450:GLN:CB	1:B:533:GLU:OE2	2.64	0.45
1:A:32:ASN:HD22	1:A:83:GLU:N	2.13	0.44
1:A:440:PRO:HB3	1:A:457:LEU:CD2	2.43	0.44
1:A:482:THR:O	1:A:483:TRP:CD2	2.70	0.44
1:B:152:LYS:O	1:B:189:LEU:HA	2.17	0.44
1:B:473:VAL:CG2	1:B:487:LEU:HD21	2.47	0.44
1:B:449:ASP:CB	1:B:532:CYS:H	2.22	0.44
1:B:440:PRO:HB3	1:B:457:LEU:CD2	2.43	0.44
1:A:187:TYR:CE1	1:A:211:ILE:HD11	2.52	0.44
1:B:299:GLN:CG	1:B:318:THR:HG23	2.42	0.44
1:B:32:ASN:ND2	1:B:83:GLU:CB	2.62	0.44
1:A:339:VAL:HG11	1:A:351:ILE:HG23	1.98	0.44
1:A:67:ASP:OD1	1:A:69:GLU:HB2	2.18	0.44
1:B:241:ARG:HE	1:B:281:ILE:CD1	2.24	0.44
1:B:232:GLU:HA	1:B:288:LEU:HD12	1.99	0.44
1:B:461:ASP:HB3	1:B:468:THR:HG22	2.00	0.44
1:B:485:ALA:O	1:B:486:GLU:OE1	2.35	0.44
1:A:374:ASP:C	1:A:375:PRO:O	2.54	0.44
1:A:461:ASP:HB3	1:A:468:THR:HG22	2.00	0.44
1:B:162:LEU:HB2	1:B:163:PHE:CE1	2.52	0.44
1:B:448:CYS:SG	1:B:537:ILE:CG2	3.01	0.44
1:B:519:ASN:O	1:B:519:ASN:CG	2.55	0.44
1:B:312:LEU:O	3:B:804:NDG:H8C1	2.17	0.44
1:A:4:ILE:HA	1:A:5:PRO:HD3	1.72	0.44
1:B:336:VAL:HG11	1:B:338:ARG:HD2	1.99	0.44
1:B:380:THR:HG22	1:B:381:VAL:N	2.32	0.44
1:B:67:ASP:OD1	1:B:69:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:SER:HA	1:B:87:PRO:HD3	1.83	0.44
1:A:381:VAL:HA	1:A:387:ILE:O	2.17	0.44
1:A:224:LYS:HE3	2:A:806:NAG:C8	2.48	0.44
1:B:117:VAL:O	1:B:212:THR:N	2.46	0.44
1:B:151:LEU:N	1:B:151:LEU:HD12	2.33	0.44
1:B:187:TYR:CE1	1:B:211:ILE:HD11	2.52	0.44
1:B:374:ASP:C	1:B:375:PRO:O	2.54	0.44
1:B:396:ARG:NH2	1:B:464:ILE:HG22	2.12	0.44
1:A:151:LEU:HD12	1:A:151:LEU:N	2.33	0.44
1:A:426:LEU:HD13	1:A:426:LEU:C	2.38	0.44
1:A:261:ILE:HD11	1:A:264:ASN:ND2	2.32	0.44
1:A:485:ALA:O	1:A:486:GLU:OE1	2.35	0.44
1:B:262:ARG:HG3	1:B:299:GLN:HB2	1.98	0.44
1:B:220:ILE:O	1:B:220:ILE:HG22	2.18	0.43
1:B:290:PHE:CD2	1:B:293:ARG:O	2.71	0.43
1:B:468:THR:C	1:B:469:TYR:O	2.54	0.43
1:A:286:LYS:C	1:A:287:GLY:O	2.55	0.43
1:A:28:LYS:CD	1:A:88:VAL:HG12	2.38	0.43
1:B:134:ASP:HB2	1:B:146:LEU:HD11	1.99	0.43
1:B:247:LEU:HD12	1:B:247:LEU:N	2.33	0.43
1:B:27:ASN:ND2	1:B:28:LYS:N	2.50	0.43
1:B:366:LYS:HG2	1:B:367:LEU:H	1.75	0.43
1:B:442:PRO:HD2	1:B:457:LEU:HD12	2.00	0.43
1:B:502:LEU:HA	1:B:502:LEU:HD23	1.82	0.43
1:B:524:VAL:HG21	2:B:904:NAG:C8	2.44	0.43
1:A:134:ASP:HB2	1:A:146:LEU:HD11	1.99	0.43
1:A:220:ILE:O	1:A:220:ILE:HG22	2.18	0.43
1:A:247:LEU:HD12	1:A:247:LEU:N	2.33	0.43
1:A:421:THR:CG2	1:A:422:GLY:N	2.81	0.43
1:B:155:PRO:CB	2:B:801:NAG:C8	2.94	0.43
1:A:35:TYR:HB3	1:B:90:GLU:CD	2.38	0.43
1:B:194:THR:HG23	1:B:201:LEU:O	2.18	0.43
1:B:297:VAL:HG21	2:B:807:NAG:H62	2.01	0.43
1:B:354:LEU:HD12	1:B:386:GLY:O	2.18	0.43
1:B:224:LYS:HE3	2:B:806:NAG:C8	2.48	0.43
1:A:232:GLU:HA	1:A:288:LEU:HD12	1.99	0.43
1:A:468:THR:C	1:A:469:TYR:O	2.54	0.43
1:A:297:VAL:HG21	2:A:807:NAG:H62	2.01	0.43
1:A:82:SER:HG	1:B:91:PRO:C	2.19	0.43
1:B:421:THR:CG2	1:B:422:GLY:N	2.81	0.43
1:B:4:ILE:HA	1:B:5:PRO:HD3	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:PHE:CD2	1:A:293:ARG:O	2.71	0.43
1:B:195:ASP:HB3	1:B:196:LEU:HG	2.01	0.43
1:A:344:ASP:CG	1:A:344:ASP:O	2.57	0.43
1:A:354:LEU:HD12	1:A:386:GLY:O	2.18	0.43
1:A:40:GLY:O	1:A:45:ASN:HB2	2.19	0.43
1:A:519:ASN:CG	1:A:519:ASN:O	2.55	0.43
1:B:1:ASP:CG	1:B:2:TRP:N	2.70	0.43
1:B:518:ASN:C	1:B:520:PRO:CD	2.87	0.43
2:A:805:NAG:H62	2:A:806:NAG:N2	2.31	0.43
1:B:239:VAL:HG13	1:B:240:GLN:N	2.34	0.43
1:A:194:THR:HG23	1:A:201:LEU:O	2.18	0.43
1:A:239:VAL:HG13	1:A:240:GLN:N	2.33	0.43
1:A:419:VAL:HG13	1:A:420:GLY:N	2.34	0.43
1:B:367:LEU:HG	1:B:367:LEU:H	1.41	0.43
1:B:419:VAL:HG13	1:B:420:GLY:N	2.34	0.43
1:B:188:THR:H	2:B:801:NAG:H83	1.84	0.43
2:B:810:NAG:O7	2:B:810:NAG:C1	2.67	0.43
1:A:264:ASN:HB3	1:A:267:GLY:HA2	2.01	0.42
1:A:347:ARG:HG3	1:A:392:GLY:N	2.33	0.42
1:B:522:LEU:HD23	1:B:522:LEU:HA	1.36	0.42
1:A:368:SER:CB	1:A:370:PHE:HE1	2.31	0.42
1:A:371:ILE:HG13	1:A:410:MET:SD	2.59	0.42
1:A:439:VAL:HA	1:A:440:PRO:HD3	1.81	0.42
1:A:32:ASN:ND2	1:A:83:GLU:CB	2.62	0.42
1:A:90:GLU:O	1:A:91:PRO:O	2.37	0.42
1:A:89:GLU:CD	1:B:1:ASP:N	2.37	0.42
1:B:22:VAL:CG2	1:B:23:GLN:N	2.81	0.42
1:B:32:ASN:HD22	1:B:83:GLU:N	2.13	0.42
1:A:154:ASP:HB3	2:A:801:NAG:C7	2.48	0.42
1:A:450:GLN:HG3	1:A:532:CYS:O	2.10	0.42
1:B:451:ASN:O	1:B:534:GLY:CA	2.60	0.42
1:A:22:VAL:CG2	1:A:23:GLN:N	2.81	0.42
1:A:347:ARG:HD2	1:A:392:GLY:CA	2.50	0.42
1:A:371:ILE:HA	1:A:410:MET:HB3	2.02	0.42
1:A:442:PRO:HD2	1:A:457:LEU:HD12	2.00	0.42
1:A:522:LEU:HB3	1:A:523:THR:H	1.57	0.42
1:B:138:ASN:C	1:B:138:ASN:ND2	2.73	0.42
1:B:261:ILE:H	1:B:261:ILE:HD13	1.85	0.42
1:B:333:VAL:HG23	1:B:334:PRO:HD3	2.01	0.42
1:B:368:SER:CB	1:B:370:PHE:HE1	2.31	0.42
1:A:298:LEU:CD2	1:A:298:LEU:N	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ILE:HD13	3:A:811:NDG:H8C3	2.01	0.42
1:A:518:ASN:C	1:A:520:PRO:CD	2.87	0.42
1:B:482:THR:HG22	1:B:499:THR:H	1.70	0.42
1:B:7:ILE:O	1:B:96:ILE:HG23	2.20	0.42
1:A:138:ASN:C	1:A:138:ASN:ND2	2.73	0.42
1:A:333:VAL:HG23	1:A:334:PRO:HD3	2.01	0.42
1:B:371:ILE:HG13	1:B:410:MET:SD	2.59	0.42
1:A:84:ASN:O	1:B:79:HIS:ND1	2.53	0.42
1:A:515:ASP:OD1	1:A:516:ALA:N	2.53	0.42
1:B:347:ARG:HD2	1:B:392:GLY:CA	2.50	0.42
1:B:441:SER:CB	1:B:442:PRO:HD3	2.47	0.42
1:B:511:VAL:N	1:B:523:THR:O	2.46	0.42
1:A:339:VAL:HG21	1:A:351:ILE:HG22	2.01	0.42
1:B:235:ILE:HG21	1:B:235:ILE:HD13	1.84	0.42
1:B:250:PRO:HA	1:B:255:TRP:CG	2.55	0.42
1:B:339:VAL:HG21	1:B:351:ILE:HG22	2.01	0.42
1:B:469:TYR:CE2	1:B:470:PRO:HD2	2.54	0.42
1:B:515:ASP:OD1	1:B:516:ALA:N	2.53	0.42
1:A:469:TYR:CE2	1:A:470:PRO:HD2	2.54	0.42
1:A:3:VAL:HB	1:A:4:ILE:H	1.51	0.42
1:A:539:CYS:HB3	1:A:540:GLN:H	1.45	0.42
1:A:524:VAL:HG21	2:A:904:NAG:C8	2.44	0.42
1:B:67:ASP:CG	1:B:69:GLU:HB2	2.40	0.42
1:B:335:ALA:HB3	3:B:811:NDG:O6	2.15	0.42
1:A:195:ASP:HB3	1:A:196:LEU:HG	2.01	0.42
1:A:441:SER:CB	1:A:442:PRO:HD3	2.47	0.42
1:B:175:ILE:CG2	1:B:176:GLY:N	2.82	0.42
1:B:230:VAL:O	1:B:323:VAL:HA	2.20	0.42
1:B:344:ASP:O	1:B:344:ASP:CG	2.57	0.42
1:B:40:GLY:O	1:B:45:ASN:HB2	2.19	0.42
1:A:108:PHE:HA	1:A:132:ALA:CB	2.50	0.41
1:A:239:VAL:HG11	1:A:282:LEU:HD22	2.02	0.41
1:A:502:LEU:HD22	1:A:503:LYS:H	1.85	0.41
1:B:108:PHE:HA	1:B:132:ALA:CB	2.50	0.41
1:B:264:ASN:HB3	1:B:267:GLY:HA2	2.01	0.41
1:B:371:ILE:HA	1:B:410:MET:HB3	2.02	0.41
1:B:514:SER:HG	1:B:519:ASN:HA	1.85	0.41
1:B:505:GLY:H	1:B:529:VAL:HB	1.85	0.41
1:A:188:THR:H	2:A:801:NAG:H83	1.84	0.41
1:A:250:PRO:HA	1:A:255:TRP:CG	2.55	0.41
2:A:810:NAG:C1	2:A:810:NAG:O7	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:VAL:HG13	1:B:128:MET:N	2.25	0.41
1:B:231:PRO:O	1:B:235:ILE:HD13	2.21	0.41
1:B:347:ARG:HG3	1:B:392:GLY:N	2.33	0.41
1:A:127:VAL:HG22	1:A:128:MET:HG3	2.03	0.41
1:A:505:GLY:H	1:A:529:VAL:HB	1.85	0.41
1:A:86:SER:HB3	1:B:92:MET:HB2	1.39	0.41
1:B:154:ASP:HB3	2:B:801:NAG:C7	2.48	0.41
1:B:231:PRO:O	1:B:288:LEU:HD12	2.20	0.41
1:B:409:ILE:HD13	3:B:811:NDG:H8C3	2.01	0.41
1:B:449:ASP:N	1:B:532:CYS:HB3	2.19	0.41
1:B:128:MET:HB3	1:B:129:ALA:H	1.62	0.41
1:A:175:ILE:CG2	1:A:176:GLY:N	2.82	0.41
1:A:42:GLY:CA	1:A:47:PRO:O	2.69	0.41
1:B:502:LEU:HD22	1:B:503:LYS:H	1.85	0.41
1:A:231:PRO:O	1:A:235:ILE:HD13	2.21	0.41
1:A:230:VAL:HG23	1:A:323:VAL:HA	2.03	0.41
1:A:230:VAL:O	1:A:323:VAL:HA	2.20	0.41
1:A:474:SER:N	1:A:512:LEU:O	2.53	0.41
1:B:230:VAL:HG23	1:B:323:VAL:HA	2.03	0.41
1:B:19:LYS:HB3	1:B:62:VAL:HG12	2.03	0.41
1:A:400:TYR:O	1:A:401:VAL:C	2.59	0.41
1:A:33:LYS:NZ	1:A:56:GLU:OE1	2.42	0.41
1:B:474:SER:N	1:B:512:LEU:O	2.53	0.41
1:A:68:ARG:HD3	1:A:100:ASP:CB	2.51	0.41
1:A:261:ILE:HD13	1:A:261:ILE:H	1.85	0.41
1:A:82:SER:OG	1:B:91:PRO:CD	2.68	0.41
1:B:108:PHE:CZ	1:B:191:VAL:HG23	2.56	0.41
1:B:68:ARG:HD3	1:B:100:ASP:CB	2.51	0.41
1:A:290:PHE:CG	1:A:292:LEU:HB2	2.56	0.41
1:A:345:LEU:HD22	1:A:349:GLU:HB2	2.03	0.41
1:A:23:GLN:HA	1:A:58:GLY:O	2.21	0.41
1:A:316:THR:OG1	2:A:806:NAG:H83	2.21	0.41
1:A:7:ILE:O	1:A:96:ILE:HG23	2.20	0.41
1:B:448:CYS:C	1:B:452:PRO:HG3	2.40	0.41
1:A:108:PHE:HA	1:A:132:ALA:HB2	2.03	0.41
1:A:138:ASN:N	1:A:138:ASN:HD22	2.19	0.41
1:A:235:ILE:HD13	1:A:235:ILE:HG21	1.84	0.41
1:A:62:VAL:HG13	1:A:62:VAL:O	2.21	0.41
1:B:25:LYS:NZ	1:B:29:ASP:OD2	2.39	0.41
1:B:373:ASN:CG	1:B:374:ASP:N	2.75	0.41
1:B:449:ASP:HB2	1:B:531:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LYS:NZ	1:B:56:GLU:OE1	2.43	0.41
1:A:193:ALA:O	1:A:202:SER:HA	2.21	0.41
1:A:297:VAL:HG22	2:A:807:NAG:H62	2.03	0.41
1:B:108:PHE:HA	1:B:132:ALA:HB2	2.03	0.41
1:B:111:ASP:O	1:B:112:VAL:HG13	2.21	0.41
1:B:193:ALA:O	1:B:202:SER:HA	2.21	0.41
1:B:319:VAL:CG1	1:B:320:THR:N	2.84	0.41
1:A:231:PRO:O	1:A:288:LEU:HD12	2.20	0.40
1:A:67:ASP:CG	1:A:69:GLU:HB2	2.40	0.40
1:B:378:TRP:HB2	1:B:379:LEU:H	1.64	0.40
2:B:805:NAG:H62	2:B:806:NAG:N2	2.31	0.40
1:A:119:GLU:CG	1:A:214:ALA:HB3	2.51	0.40
1:A:409:ILE:HD13	3:A:811:NDG:C8	2.51	0.40
1:A:23:GLN:HB2	1:A:59:TRP:CD2	2.55	0.40
1:B:540:GLN:NE2	1:B:540:GLN:O	2.47	0.40
1:B:316:THR:OG1	2:B:806:NAG:H83	2.21	0.40
1:A:108:PHE:CZ	1:A:191:VAL:HG23	2.56	0.40
1:A:373:ASN:CG	1:A:374:ASP:N	2.75	0.40
1:A:466:PRO:O	1:A:469:TYR:N	2.46	0.40
1:B:127:VAL:HG22	1:B:128:MET:HG3	2.03	0.40
1:B:239:VAL:HG11	1:B:282:LEU:HD22	2.02	0.40
1:B:272:THR:O	1:B:281:ILE:HG22	2.21	0.40
1:B:400:TYR:O	1:B:401:VAL:C	2.59	0.40
1:A:249:MET:HA	1:A:250:PRO:HD3	1.85	0.40
1:A:319:VAL:CG1	1:A:320:THR:N	2.84	0.40
1:A:371:ILE:HA	1:A:371:ILE:HD12	1.65	0.40
1:A:423:THR:CG2	2:A:810:NAG:N2	2.84	0.40
1:B:23:GLN:HA	1:B:58:GLY:O	2.21	0.40
1:B:23:GLN:HB2	1:B:59:TRP:CD2	2.55	0.40
1:B:298:LEU:N	1:B:298:LEU:CD2	2.75	0.40
1:B:396:ARG:HH21	1:B:432:ASP:CG	2.25	0.40
1:A:28:LYS:NZ	1:B:4:ILE:HG22	2.37	0.40
1:B:423:THR:CG2	2:B:810:NAG:N2	2.84	0.40
1:A:111:ASP:O	1:A:112:VAL:HG13	2.21	0.40
1:B:432:ASP:CG	1:B:433:VAL:N	2.74	0.40
1:B:409:ILE:HD13	3:B:811:NDG:C8	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	15
1	B	538/880 (61%)	401 (74%)	92 (17%)	45 (8%)	1	15
All	All	1076/1760 (61%)	802 (74%)	184 (17%)	90 (8%)	2	15

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	PRO
1	A	155	PRO
1	A	235	ILE
1	A	347	ARG
1	A	363	GLN
1	A	364	ILE
1	A	374	ASP
1	A	404	ASN
1	A	467	ASN
1	A	476	SER
1	A	502	LEU
1	A	517	GLN
1	A	518	ASN
1	A	519	ASN
1	B	91	PRO
1	B	155	PRO
1	B	235	ILE
1	B	347	ARG
1	B	363	GLN
1	B	364	ILE
1	B	374	ASP
1	B	404	ASN
1	B	467	ASN
1	B	476	SER
1	B	502	LEU

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Mol	Chain	Res	Type
1	B	517	GLN
1	B	518	ASN
1	B	519	ASN
1	A	3	VAL
1	A	156	GLU
1	A	260	LYS
1	A	287	GLY
1	A	470	PRO
1	A	503	LYS
1	B	3	VAL
1	B	156	GLU
1	B	260	LYS
1	B	287	GLY
1	B	470	PRO
1	B	503	LYS
1	A	55	TRP
1	A	212	THR
1	A	250	PRO
1	A	333	VAL
1	A	360	ASP
1	A	372	GLY
1	A	377	ARG
1	A	506	ASP
1	B	55	TRP
1	B	212	THR
1	B	250	PRO
1	B	333	VAL
1	B	360	ASP
1	B	372	GLY
1	B	377	ARG
1	B	506	ASP
1	A	152	LYS
1	A	223	PRO
1	A	359	PRO
1	A	375	PRO
1	B	152	LYS
1	B	223	PRO
1	B	359	PRO
1	B	375	PRO
1	A	160	PRO
1	A	265	GLU
1	A	278	ASN

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Mol	Chain	Res	Type
1	A	289	ASP
1	A	482	THR
1	B	160	PRO
1	B	265	GLU
1	B	278	ASN
1	B	289	ASP
1	B	482	THR
1	A	498	PRO
1	A	523	THR
1	B	498	PRO
1	B	523	THR
1	A	154	ASP
1	A	307	PRO
1	B	154	ASP
1	B	307	PRO
1	A	222	ASP
1	B	222	ASP
1	A	200	GLY
1	B	200	GLY
1	A	47	PRO
1	A	158	PRO
1	B	47	PRO
1	B	158	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	480/779 (62%)	381 (79%)	99 (21%)	1	8
1	B	480/779 (62%)	381 (79%)	99 (21%)	1	8
All	All	960/1558 (62%)	762 (79%)	198 (21%)	4	8

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	18	PRO
1	A	19	LYS
1	A	27	ASN
1	A	52	ARG
1	A	61	LEU
1	A	66	LEU
1	A	68	ARG
1	A	88	VAL
1	A	91	PRO
1	A	92	MET
1	A	117	VAL
1	A	138	ASN
1	A	146	LEU
1	A	151	LEU
1	A	155	PRO
1	A	156	GLU
1	A	161	ASN
1	A	163	PHE
1	A	189	LEU
1	A	195	ASP
1	A	202	SER
1	A	216	ASP
1	A	217	ASN
1	A	223	PRO
1	A	226	TYR
1	A	231	PRO
1	A	233	ASN
1	A	234	GLU
1	A	235	ILE
1	A	237	PHE
1	A	250	PRO
1	A	253	PRO
1	A	261	ILE
1	A	264	ASN
1	A	268	PHE
1	A	273	THR
1	A	277	SER
1	A	278	ASN
1	A	282	LEU
1	A	284	THR
1	A	288	LEU
1	A	298	LEU

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Mol	Chain	Res	Type
1	A	309	SER
1	A	310	VAL
1	A	315	SER
1	A	316	THR
1	A	318	THR
1	A	333	VAL
1	A	336	VAL
1	A	339	VAL
1	A	345	LEU
1	A	353	SER
1	A	354	LEU
1	A	360	ASP
1	A	363	GLN
1	A	364	ILE
1	A	365	GLN
1	A	371	ILE
1	A	373	ASN
1	A	375	PRO
1	A	379	LEU
1	A	382	ASN
1	A	384	ASP
1	A	385	ASN
1	A	393	ASN
1	A	394	LEU
1	A	395	ASP
1	A	398	SER
1	A	399	GLU
1	A	404	ASN
1	A	405	THR
1	A	407	THR
1	A	410	MET
1	A	423	THR
1	A	425	THR
1	A	427	ILE
1	A	428	LEU
1	A	433	VAL
1	A	436	ASN
1	A	447	MET
1	A	448	CYS
1	A	461	ASP
1	A	464	ILE
1	A	465	PRO

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Mol	Chain	Res	Type
1	A	466	PRO
1	A	470	PRO
1	A	477	HIS
1	A	492	THR
1	A	509	ILE
1	A	512	LEU
1	A	517	GLN
1	A	518	ASN
1	A	519	ASN
1	A	520	PRO
1	A	522	LEU
1	A	523	THR
1	A	532	CYS
1	A	540	GLN
1	B	8	LYS
1	B	18	PRO
1	B	19	LYS
1	B	27	ASN
1	B	52	ARG
1	B	61	LEU
1	B	66	LEU
1	B	68	ARG
1	B	88	VAL
1	B	91	PRO
1	B	92	MET
1	B	117	VAL
1	B	138	ASN
1	B	146	LEU
1	B	151	LEU
1	B	155	PRO
1	B	156	GLU
1	B	161	ASN
1	B	163	PHE
1	B	189	LEU
1	B	195	ASP
1	B	202	SER
1	B	216	ASP
1	B	217	ASN
1	B	223	PRO
1	B	226	TYR
1	B	231	PRO
1	B	233	ASN

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Mol	Chain	Res	Type
1	B	234	GLU
1	B	235	ILE
1	B	237	PHE
1	B	250	PRO
1	B	253	PRO
1	B	261	ILE
1	B	264	ASN
1	B	268	PHE
1	B	273	THR
1	B	277	SER
1	B	278	ASN
1	B	282	LEU
1	B	284	THR
1	B	288	LEU
1	B	298	LEU
1	B	309	SER
1	B	310	VAL
1	B	315	SER
1	B	316	THR
1	B	318	THR
1	B	333	VAL
1	B	336	VAL
1	B	339	VAL
1	B	345	LEU
1	B	353	SER
1	B	354	LEU
1	B	360	ASP
1	B	363	GLN
1	B	364	ILE
1	B	365	GLN
1	B	371	ILE
1	B	373	ASN
1	B	375	PRO
1	B	379	LEU
1	B	382	ASN
1	B	384	ASP
1	B	385	ASN
1	B	393	ASN
1	B	394	LEU
1	B	395	ASP
1	B	398	SER
1	B	399	GLU

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Mol	Chain	Res	Type
1	B	404	ASN
1	B	405	THR
1	B	407	THR
1	B	410	MET
1	B	423	THR
1	B	425	THR
1	B	427	ILE
1	B	428	LEU
1	B	433	VAL
1	B	436	ASN
1	B	447	MET
1	B	448	CYS
1	B	461	ASP
1	B	464	ILE
1	B	465	PRO
1	B	466	PRO
1	B	470	PRO
1	B	477	HIS
1	B	492	THR
1	B	509	ILE
1	B	512	LEU
1	B	517	GLN
1	B	518	ASN
1	B	519	ASN
1	B	520	PRO
1	B	522	LEU
1	B	523	THR
1	B	532	CYS
1	B	540	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	27	ASN
1	A	32	ASN
1	A	45	ASN
1	A	104	ASN
1	A	110	GLN
1	A	122	GLN
1	A	138	ASN
1	A	217	ASN

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Mol	Chain	Res	Type
1	A	233	ASN
1	A	240	GLN
1	A	264	ASN
1	A	278	ASN
1	A	299	GLN
1	A	373	ASN
1	A	385	ASN
1	A	391	ASN
1	A	393	ASN
1	A	404	ASN
1	A	455	GLN
1	A	467	ASN
1	A	517	GLN
1	A	519	ASN
1	B	12	ASN
1	B	27	ASN
1	B	32	ASN
1	B	45	ASN
1	B	79	HIS
1	B	104	ASN
1	B	110	GLN
1	B	122	GLN
1	B	138	ASN
1	B	217	ASN
1	B	233	ASN
1	B	240	GLN
1	B	264	ASN
1	B	278	ASN
1	B	299	GLN
1	B	373	ASN
1	B	385	ASN
1	B	391	ASN
1	B	393	ASN
1	B	404	ASN
1	B	455	GLN
1	B	467	ASN
1	B	517	GLN
1	B	519	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 24 are monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	801	1	14,14,15	0.67	0	15,19,21	0.99	1 (6%)
2	NAG	A	802	1	14,14,15	0.73	0	15,19,21	0.92	0
2	NAG	A	803	1	14,14,15	0.94	1 (7%)	15,19,21	1.20	2 (13%)
3	NDG	A	804	1	14,14,15	0.63	0	15,19,21	0.82	0
2	NAG	A	805	1	14,14,15	0.69	0	15,19,21	1.07	1 (6%)
2	NAG	A	806	1	14,14,15	0.55	0	15,19,21	1.44	3 (20%)
2	NAG	A	807	1	14,14,15	0.65	0	15,19,21	1.25	2 (13%)
2	NAG	A	808	1	14,14,15	0.66	0	15,19,21	0.68	0
2	NAG	A	809	1	14,14,15	0.76	1 (7%)	15,19,21	0.86	0
2	NAG	A	810	1	14,14,15	0.65	0	15,19,21	1.40	4 (26%)
3	NDG	A	811	1	14,14,15	0.86	0	15,19,21	1.95	1 (6%)
2	NAG	A	812	1	14,14,15	0.84	1 (7%)	15,19,21	0.75	1 (6%)
3	NDG	A	902	1	14,14,15	1.10	1 (7%)	15,19,21	1.14	1 (6%)
3	NDG	A	903	1	14,14,15	0.52	0	15,19,21	0.80	0
2	NAG	A	904	1	14,14,15	0.77	1 (7%)	15,19,21	0.64	0
2	NAG	B	801	1	14,14,15	0.66	0	15,19,21	1.00	1 (6%)
2	NAG	B	802	1	14,14,15	0.74	0	15,19,21	0.91	0
2	NAG	B	803	1	14,14,15	0.94	1 (7%)	15,19,21	1.21	2 (13%)
3	NDG	B	804	1	14,14,15	0.62	0	15,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	805	1	14,14,15	0.70	0	15,19,21	1.07	1 (6%)
2	NAG	B	806	1	14,14,15	0.55	0	15,19,21	1.45	3 (20%)
2	NAG	B	807	1	14,14,15	0.64	0	15,19,21	1.25	2 (13%)
2	NAG	B	808	1	14,14,15	0.68	0	15,19,21	0.67	0
2	NAG	B	809	1	14,14,15	0.77	1 (7%)	15,19,21	0.86	0
2	NAG	B	810	1	14,14,15	0.64	0	15,19,21	1.40	4 (26%)
3	NDG	B	811	1	14,14,15	0.84	0	15,19,21	1.96	1 (6%)
2	NAG	B	812	1	14,14,15	0.85	1 (7%)	15,19,21	0.75	0
3	NDG	B	902	1	14,14,15	1.09	1 (7%)	15,19,21	1.14	1 (6%)
3	NDG	B	903	1	14,14,15	0.52	0	15,19,21	0.80	0
2	NAG	B	904	1	14,14,15	0.77	1 (7%)	15,19,21	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
2	NAG	A	802	1	-	0/6/23/26	0/1/1/1
2	NAG	A	803	1	-	0/6/23/26	0/1/1/1
3	NDG	A	804	1	-	0/6/23/26	0/1/1/1
2	NAG	A	805	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	806	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	807	1	-	0/6/23/26	0/1/1/1
2	NAG	A	808	1	-	0/6/23/26	0/1/1/1
2	NAG	A	809	1	-	0/6/23/26	0/1/1/1
2	NAG	A	810	1	-	0/6/23/26	0/1/1/1
3	NDG	A	811	1	-	0/6/23/26	0/1/1/1
2	NAG	A	812	1	-	0/6/23/26	0/1/1/1
3	NDG	A	902	1	-	0/6/23/26	0/1/1/1
3	NDG	A	903	1	-	0/6/23/26	0/1/1/1
2	NAG	A	904	1	-	0/6/23/26	0/1/1/1
2	NAG	B	801	1	-	0/6/23/26	0/1/1/1
2	NAG	B	802	1	-	0/6/23/26	0/1/1/1
2	NAG	B	803	1	-	0/6/23/26	0/1/1/1
3	NDG	B	804	1	-	0/6/23/26	0/1/1/1
2	NAG	B	805	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	806	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	807	1	-	0/6/23/26	0/1/1/1
2	NAG	B	808	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	809	1	-	0/6/23/26	0/1/1/1
2	NAG	B	810	1	-	0/6/23/26	0/1/1/1
3	NDG	B	811	1	-	0/6/23/26	0/1/1/1
2	NAG	B	812	1	-	0/6/23/26	0/1/1/1
3	NDG	B	902	1	-	0/6/23/26	0/1/1/1
3	NDG	B	903	1	-	0/6/23/26	0/1/1/1
2	NAG	B	904	1	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	904	NAG	C1-C2	-2.44	1.49	1.52
2	A	904	NAG	C1-C2	-2.42	1.49	1.52
2	B	812	NAG	C1-C2	-2.37	1.49	1.52
2	A	812	NAG	C1-C2	-2.36	1.49	1.52
2	B	809	NAG	C1-C2	-2.05	1.49	1.52
2	A	809	NAG	C1-C2	-2.01	1.49	1.52
2	A	803	NAG	O5-C5	2.42	1.48	1.43
2	B	803	NAG	O5-C5	2.42	1.48	1.43
3	B	902	NDG	C1-C2	3.20	1.56	1.52
3	A	902	NDG	C1-C2	3.27	1.57	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	811	NDG	C2-N2-C7	-6.87	112.92	122.94
3	A	811	NDG	C2-N2-C7	-6.85	112.95	122.94
2	A	806	NAG	C2-N2-C7	-3.36	118.04	122.94
2	B	806	NAG	C2-N2-C7	-3.35	118.05	122.94
2	B	805	NAG	C2-N2-C7	-2.97	118.61	122.94
2	A	805	NAG	C2-N2-C7	-2.94	118.66	122.94
2	B	807	NAG	C2-N2-C7	-2.83	118.81	122.94
2	A	807	NAG	C2-N2-C7	-2.83	118.82	122.94
2	A	810	NAG	O5-C1-C2	-2.78	107.60	111.47
2	B	810	NAG	O5-C1-C2	-2.78	107.61	111.47
2	A	803	NAG	C2-N2-C7	-2.75	118.93	122.94
2	B	803	NAG	C2-N2-C7	-2.75	118.94	122.94
2	B	810	NAG	C4-C3-C2	-2.46	107.41	111.02
2	A	810	NAG	C4-C3-C2	-2.45	107.42	111.02
2	B	807	NAG	O5-C1-C2	-2.45	108.06	111.47
2	A	806	NAG	C4-C3-C2	-2.45	107.43	111.02
2	B	806	NAG	C4-C3-C2	-2.44	107.44	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	807	NAG	O5-C1-C2	-2.43	108.08	111.47
2	B	806	NAG	O5-C1-C2	-2.39	108.15	111.47
2	A	806	NAG	O5-C1-C2	-2.38	108.17	111.47
2	B	810	NAG	C1-O5-C5	-2.17	109.17	112.17
2	A	810	NAG	C1-O5-C5	-2.16	109.19	112.17
2	A	812	NAG	C2-N2-C7	-2.01	120.01	122.94
2	A	801	NAG	C1-C2-N2	-2.00	107.07	110.49
2	B	801	NAG	C1-C2-N2	-2.00	107.07	110.49
3	A	902	NDG	O-C1-C2	2.27	114.63	111.47
2	B	810	NAG	C1-C2-N2	2.28	114.38	110.49
3	B	902	NDG	O-C1-C2	2.28	114.65	111.47
2	A	810	NAG	C1-C2-N2	2.30	114.41	110.49
2	A	803	NAG	C1-O5-C5	2.37	115.44	112.17
2	B	803	NAG	C1-O5-C5	2.38	115.45	112.17

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	806	NAG	C1
2	A	806	NAG	C1
2	B	805	NAG	C1
2	A	805	NAG	C1

There are no torsion outliers.

There are no ring outliers.

26 monomers are involved in 202 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAG	21	0
2	A	803	NAG	4	0
3	A	804	NDG	2	0
2	A	805	NAG	7	0
2	A	806	NAG	12	0
2	A	807	NAG	17	0
2	A	808	NAG	2	0
2	A	809	NAG	8	0
2	A	810	NAG	13	0
3	A	811	NDG	6	0
2	A	812	NAG	3	0
3	A	902	NDG	8	0
2	A	904	NAG	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	NAG	21	0
2	B	803	NAG	4	0
3	B	804	NDG	2	0
2	B	805	NAG	7	0
2	B	806	NAG	12	0
2	B	807	NAG	16	0
2	B	808	NAG	2	0
2	B	809	NAG	8	0
2	B	810	NAG	13	0
3	B	811	NDG	7	0
2	B	812	NAG	3	0
3	B	902	NDG	8	0
2	B	904	NAG	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.