



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 8, 2017 – 12:16 PM EST

PDB ID : 5MKE  
EMDB ID: : EMD-3523  
Title : cryoEM Structure of Polycystin-2 in complex with cations and lipids  
Authors : Wilkes, M.; Madej, M.G.; Ziegler, C.  
Deposited on : 2016-12-04  
Resolution : 4.30 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](mailto: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.

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

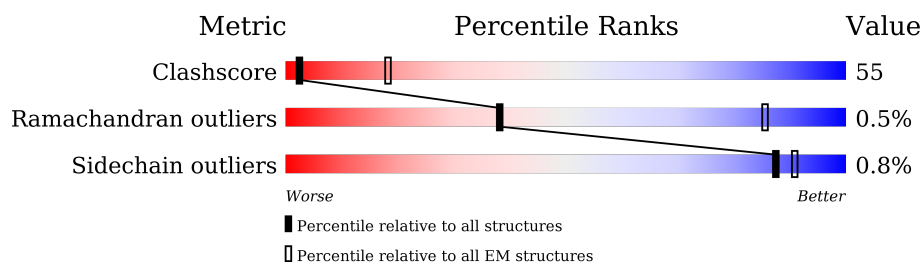
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	968	
1	B	968	
1	C	968	
1	D	968	

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	1002	-	-	X	-
2	NAG	B	1002	-	-	X	-
2	NAG	C	1002	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	1002	-	-	X	-

## 2 Entry composition [i](#)

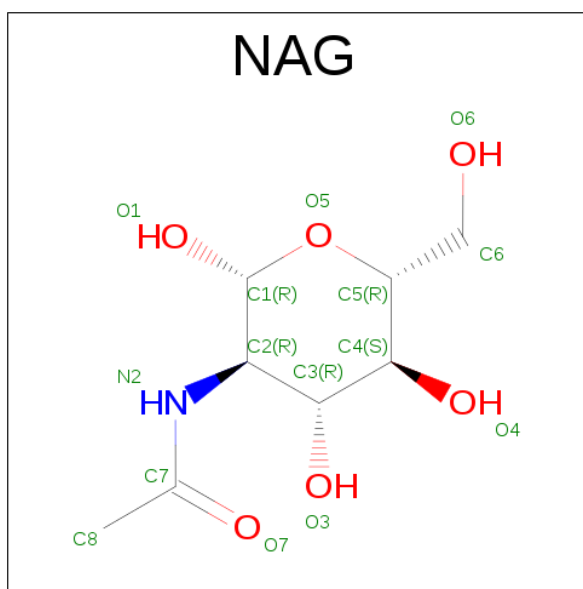
There are 6 unique types of molecules in this entry. The entry contains 16426 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Polycystin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	475	Total	C	N	O	S	0	0
			3926	2595	621	691	19		
1	B	475	Total	C	N	O	S	0	0
			3926	2595	621	691	19		
1	C	475	Total	C	N	O	S	0	0
			3926	2595	621	691	19		
1	D	475	Total	C	N	O	S	0	0
			3926	2595	621	691	19		

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



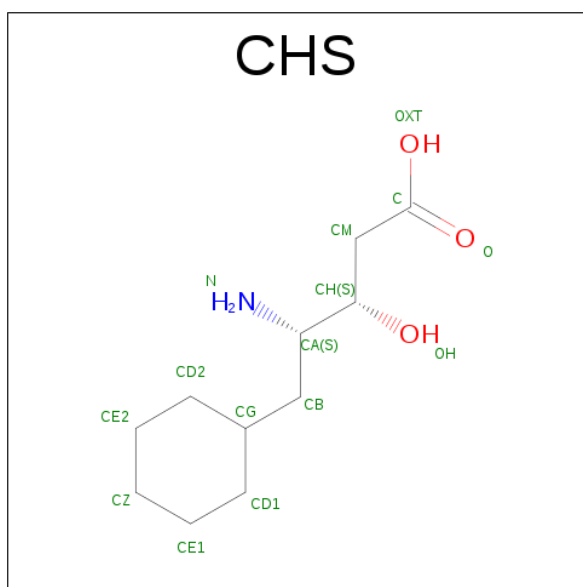
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			56	32	4	20	
2	A	1	Total	C	N	O	0
			56	32	4	20	
2	A	1	Total	C	N	O	0
			56	32	4	20	

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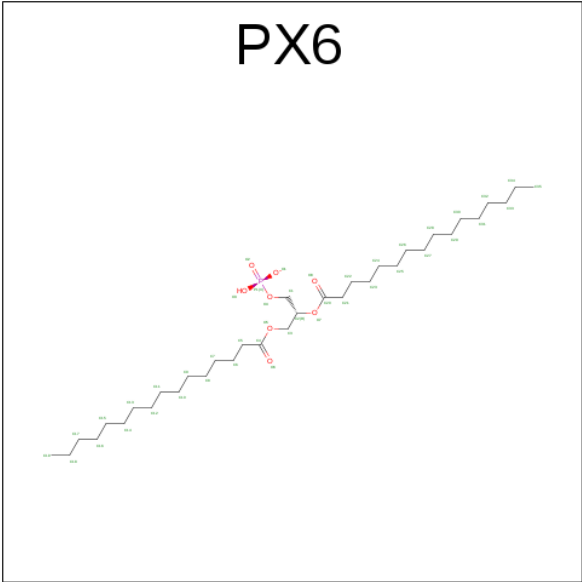
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			56	32	4	20	
2	B	1	Total	C	N	O	0
			56	32	4	20	
2	B	1	Total	C	N	O	0
			56	32	4	20	
2	B	1	Total	C	N	O	0
			56	32	4	20	
2	B	1	Total	C	N	O	0
			56	32	4	20	
2	C	1	Total	C	N	O	0
			56	32	4	20	
2	C	1	Total	C	N	O	0
			56	32	4	20	
2	C	1	Total	C	N	O	0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

- Molecule 3 is 4-AMINO-5-CYCLOHEXYL-3-HYDROXY-PENTANOIC ACID (three-letter code: CHS) (formula: C<sub>11</sub>H<sub>21</sub>NO<sub>3</sub>).



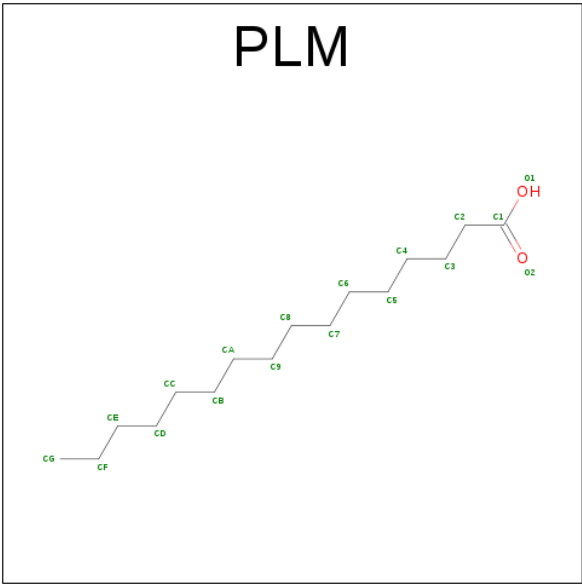
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			30	22	2	6	
3	A	1	Total	C	N	O	0
			30	22	2	6	
3	B	1	Total	C	N	O	0
			30	22	2	6	
3	B	1	Total	C	N	O	0
			30	22	2	6	
3	C	1	Total	C	N	O	0
			30	22	2	6	
3	C	1	Total	C	N	O	0
			30	22	2	6	
3	D	1	Total	C	N	O	0
			30	22	2	6	
3	D	1	Total	C	N	O	0
			30	22	2	6	

- Molecule 4 is 1,2-DIPALMITOYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX6) (formula: C<sub>35</sub>H<sub>68</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			40	31	8	1	
4	B	1	Total	C	O	P	0
			40	31	8	1	
4	C	1	Total	C	O	P	0
			40	31	8	1	
4	D	1	Total	C	O	P	0
			40	31	8	1	

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			54	48	6	
5	A	1	Total	C	O	0
			54	48	6	
5	A	1	Total	C	O	0
			54	48	6	
5	B	1	Total	C	O	0
			54	48	6	
5	B	1	Total	C	O	0
			54	48	6	
5	B	1	Total	C	O	0
			54	48	6	
5	C	1	Total	C	O	0
			54	48	6	
5	C	1	Total	C	O	0
			54	48	6	
5	C	1	Total	C	O	0
			54	48	6	
5	D	1	Total	C	O	0
			54	48	6	
5	D	1	Total	C	O	0
			54	48	6	
5	D	1	Total	C	O	0
			54	48	6	

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

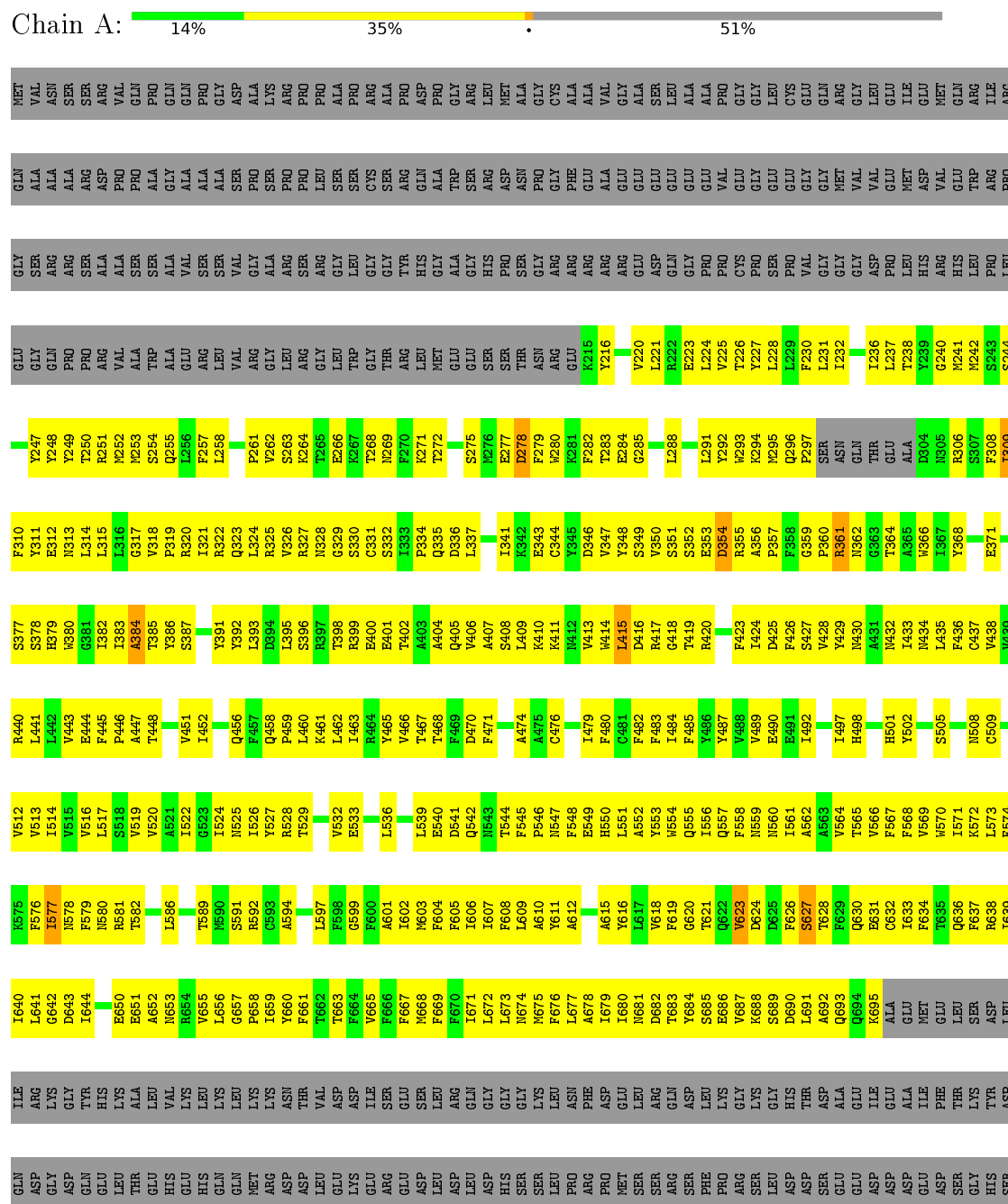
Mol	Chain	Residues	Atoms		AltConf
6	A	2	Total	Ca	0
			2	2	



### 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 errors 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: Polycystin-2



Chain B:  13% 34% . 51%



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

- Molecule 1: Polycystin-2

Chain C:  14% 35% . 51%

MET	VAL	ASN	SER	SER	ARG	VAL	GLN	PRO	GLN	GLN	PRO	GLY	ASP	ALA	LYS	ARG	PRO	PRO	ALA	ALA	PRO	ARG	ARG	ALA	PRO	ASP	PRO	GLY	GLY	CYS	ALA	ALA	VAL	GLY	ALA	SER	SER	LEU	LEU	CYS	GLU	GLU	ARG	GLN	ILE	ILE	PCP
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[illegible]

GLY	SER	ARG	ARG	SER	ALA	ALA	SER	SER	ALA	VAL	SER	SER	VAL	GLY	ALA	ARG	SER	ARG	GLY	LEU	GLY	TYR	HIS	ALA	GLY	HIS	PRO	SER	GLY	ARG	ARG	ARG	ARG	GLU	ASP	GLN	GLY	PRO	PRO	CYS	PRO	SER	PRO	PRO	VAL	GLY	GLY	GLY	ASP	PRO	LEU	HIS	HIS	LEU	PRO	LEU
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GLU	GLN	GLY	PRO	PRO	ARG	VAL	TRP	ALA	ALA	GLU	ARG	LEU	VAL	ARG	GLY	GLY	THR	ARG	LEU	ARG	GLY	TRP	GLU	GLU	SER	SER	THR	ASN	ARG	GLU	<b>Z215</b>	<b>Z216</b>	Z220	Z221	<b>Z222</b>	<b>Z223</b>	Z224	Z225	Z226	Z227	Z228	<b>Z229</b>	Z230	Z231	<b>Z232</b>	Z236	Z237	Z238	<b>Z239</b>	Z240	M241	M242	<b>Z243</b>	<b>Z244</b>
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[illegible][illegible]

S378	R379	R380	<b>S381</b>	<b>S382</b>	<b>S383</b>	<b>S384</b>	R385	R386	<b>S387</b>	<b>S389</b>	R392	R393	<b>S394</b>	R395	<b>S396</b>	R397	R398	R399	<b>E400</b>	<b>E401</b>	<b>T402</b>	<b>A403</b>	<b>A404</b>	<b>Q405</b>	<b>V406</b>	<b>A407</b>	<b>S408</b>	<b>L409</b>	<b>K410</b>	<b>K411</b>	<b>M412</b>	<b>V413</b>	<b>K414</b>	<b>L415</b>	<b>D416</b>	<b>R417</b>	<b>G418</b>	<b>T419</b>	<b>R420</b>	<b>F423</b>	<b>I424</b>	<b>D425</b>	<b>F426</b>	<b>S427</b>	<b>V428</b>	<b>V429</b>	<b>M430</b>	<b>A431</b>	<b>M432</b>	<b>I433</b>	<b>M434</b>	<b>L435</b>	<b>F436</b>	<b>C437</b>	<b>V438</b>	<b>W439</b>	<b>M440</b>
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I441	I442	I443	E444	F445	F446	A447	I448	I451	I452	F456	F457	Q458	P459	L460	L461	L462	L463	L464	F465	V466	T467	T468	F469	D470	F471	A474	A475	C476	I479	F480	C481	F482	F483	L484	L485	F486	F487	L488	V489	E490	F503	F504	R505	S506	N508	C509
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V512	V513	V514	V515	V516	V517	V518	V519	V520	V521	V522	V523	V524	V525	V526	V527	V528	V529	V530	V531	V532	V533	V534	V535	V536	V537	V538	V539	V540	V541	V542	V543	V544	V545	V546	V547	V548	V549	V550	V551	V552	V553	V554	V555	V556	V557	V558	V559	V560	V561	V562	V563	V564	V565	V566	V567	V568	V569	V570	V571	V572	V573	V574	V575	V576	V577	V578	V579	V580	V581	V582	V583	V584	V585	V586	V587	V588	V589	V590	V591	V592	V593	V594	V595	V596	V597	V598	V599	V600	V601	V602	V603	V604	V605	V606	V607	V608	V609	V610	V611	V612	V613	V614	V615	V616	V617	V618	V619	V620	V621	V622	V623	V624	V625	V626	V627	V628	V629	V630	V631	V632	V633	V634	V635	V636	V637	V638	V639	V640	V641	V642	V643	V644	V645	V646	V647	V648	V649	V650	V651	V652	V653	V654	V655	V656	V657	V658	V659	V660	V661	V662	V663	V664	V665	V666	V667	V668	V669	V670	V671	V672	V673	V674	V675	V676	V677	V678	V679	V680	V681	V682	V683	V684	V685	V686	V687	V688	V689	V690	V691	V692	V693	V694	V695	V696	V697	V698	V699	V700	V701	V702	V703	V704	V705	V706	V707	V708	V709	V710	V711	V712	V713	V714	V715	V716	V717	V718	V719	V720	V721	V722	V723	V724	V725	V726	V727	V728	V729	V730	V731	V732	V733	V734	V735	V736	V737	V738	V739	V740	V741	V742	V743	V744	V745	V746	V747	V748	V749	V750	V751	V752	V753	V754	V755	V756	V757	V758	V759	V760	V761	V762	V763	V764	V765	V766	V767	V768	V769	V770	V771	V772	V773	V774	V775	V776	V777	V778	V779	V780	V781	V782	V783	V784	V785	V786	V787	V788	V789	V790	V791	V792	V793	V794	V795	V796	V797	V798	V799	V800	V801	V802	V803	V804	V805	V806	V807	V808	V809	V810	V811	V812	V813	V814	V815	V816	V817	V818	V819	V820	V821	V822	V823	V824	V825	V826	V827	V828	V829	V830	V831	V832	V833	V834	V835	V836	V837	V838	V839	V840	V841	V842	V843	V844	V845	V846	V847	V848	V849	V850	V851	V852	V853	V854	V855	V856	V857	V858	V859	V860	V861	V862	V863	V864	V865	V866	V867	V868	V869	V870	V871	V872	V873	V874	V875	V876	V877	V878	V879	V880	V881	V882	V883	V884	V885	V886	V887	V888	V889	V890	V891	V892	V893	V894	V895	V896	V897	V898	V899	V900	V901	V902	V903	V904	V905	V906	V907	V908	V909	V910	V911	V912	V913	V914	V915	V916	V917	V918	V919	V920	V921	V922	V923	V924	V925	V926	V927	V928	V929	V930	V931	V932	V933	V934	V935	V936	V937	V938	V939	V940	V941	V942	V943	V944	V945	V946	V947	V948	V949	V950	V951	V952	V953	V954	V955	V956	V957	V958	V959	V960	V961	V962	V963	V964	V965	V966	V967	V968	V969	V970	V971	V972	V973	V974	V975	V976	V977	V978	V979	V980	V981	V982	V983	V984	V985	V986	V987	V988	V989	V990	V991	V992	V993	V994	V995	V996	V997	V998	V999	V1000
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<b>F575</b>	<b>F576</b>	<b>F577</b>	<b>F578</b>	<b>F579</b>	<b>F580</b>	<b>F581</b>	<b>F582</b>	<b>F586</b>	<b>F589</b>	<b>F590</b>	<b>F591</b>	<b>F592</b>	<b>F593</b>	<b>F594</b>	<b>F595</b>	<b>F596</b>	<b>F597</b>	<b>F598</b>	<b>F599</b>	<b>F600</b>	<b>F601</b>	<b>F602</b>	<b>F603</b>	<b>F604</b>	<b>F605</b>	<b>F606</b>	<b>F607</b>	<b>F608</b>	<b>F609</b>	<b>F610</b>	<b>F611</b>	<b>F612</b>	<b>F615</b>	<b>F616</b>	<b>F617</b>	<b>F618</b>	<b>F619</b>	<b>F620</b>	<b>F621</b>	<b>F622</b>	<b>F623</b>	<b>F624</b>	<b>F625</b>	<b>F626</b>	<b>F627</b>	<b>F628</b>	<b>F629</b>	<b>F630</b>	<b>F631</b>	<b>F632</b>	<b>F633</b>	<b>F634</b>	<b>F635</b>	<b>F636</b>	<b>F637</b>	<b>F638</b>	<b>F639</b>	<b>F640</b>	<b>F641</b>	<b>F642</b>	<b>F643</b>	<b>F644</b>	<b>F645</b>	<b>F646</b>	<b>F647</b>	<b>F648</b>	<b>F649</b>	<b>F650</b>	<b>F651</b>	<b>F652</b>	<b>F653</b>	<b>F654</b>	<b>F655</b>	<b>F656</b>	<b>F657</b>	<b>F658</b>	<b>F659</b>	<b>F660</b>	<b>F661</b>	<b>F662</b>	<b>F663</b>	<b>F664</b>	<b>F665</b>	<b>F666</b>	<b>F667</b>	<b>F668</b>	<b>F669</b>	<b>F670</b>	<b>F671</b>	<b>F672</b>	<b>F673</b>	<b>F674</b>	<b>F675</b>	<b>F676</b>	<b>F677</b>	<b>F678</b>	<b>F679</b>	<b>F680</b>	<b>F681</b>	<b>F682</b>	<b>F683</b>	<b>F684</b>	<b>F685</b>	<b>F686</b>	<b>F687</b>	<b>F688</b>	<b>F689</b>	<b>F690</b>	<b>F691</b>	<b>F692</b>	<b>F693</b>	<b>F694</b>	<b>F695</b>	<b>F696</b>	<b>F697</b>	<b>F698</b>	<b>F699</b>	<b>F700</b>	<b>F701</b>	<b>F702</b>	<b>F703</b>	<b>F704</b>	<b>F705</b>	<b>F706</b>	<b>F707</b>	<b>F708</b>	<b>F709</b>	<b>F710</b>	<b>F711</b>	<b>F712</b>	<b>F713</b>	<b>F714</b>	<b>F715</b>	<b>F716</b>	<b>F717</b>	<b>F718</b>	<b>F719</b>	<b>F720</b>	<b>F721</b>	<b>F722</b>	<b>F723</b>	<b>F724</b>	<b>F725</b>	<b>F726</b>	<b>F727</b>	<b>F728</b>	<b>F729</b>	<b>F730</b>	<b>F731</b>	<b>F732</b>	<b>F733</b>	<b>F734</b>	<b>F735</b>	<b>F736</b>	<b>F737</b>	<b>F738</b>	<b>F739</b>	<b>F740</b>	<b>F741</b>	<b>F742</b>	<b>F743</b>	<b>F744</b>	<b>F745</b>	<b>F746</b>	<b>F747</b>	<b>F748</b>	<b>F749</b>	<b>F750</b>	<b>F751</b>	<b>F752</b>	<b>F753</b>	<b>F754</b>	<b>F755</b>	<b>F756</b>	<b>F757</b>	<b>F758</b>	<b>F759</b>	<b>F760</b>	<b>F761</b>	<b>F762</b>	<b>F763</b>	<b>F764</b>	<b>F765</b>	<b>F766</b>	<b>F767</b>	<b>F768</b>	<b>F769</b>	<b>F770</b>	<b>F771</b>	<b>F772</b>	<b>F773</b>	<b>F774</b>	<b>F775</b>	<b>F776</b>	<b>F777</b>	<b>F778</b>	<b>F779</b>	<b>F780</b>	<b>F781</b>	<b>F782</b>	<b>F783</b>	<b>F784</b>	<b>F785</b>	<b>F786</b>	<b>F787</b>	<b>F788</b>	<b>F789</b>	<b>F790</b>	<b>F791</b>	<b>F792</b>	<b>F793</b>	<b>F794</b>	<b>F795</b>	<b>F796</b>	<b>F797</b>	<b>F798</b>	<b>F799</b>	<b>F800</b>	<b>F801</b>	<b>F802</b>	<b>F803</b>	<b>F804</b>	<b>F805</b>	<b>F806</b>	<b>F807</b>	<b>F808</b>	<b>F809</b>	<b>F810</b>	<b>F811</b>	<b>F812</b>	<b>F813</b>	<b>F814</b>	<b>F815</b>	<b>F816</b>	<b>F817</b>	<b>F818</b>	<b>F819</b>	<b>F820</b>	<b>F821</b>	<b>F822</b>	<b>F823</b>	<b>F824</b>	<b>F825</b>	<b>F826</b>	<b>F827</b>	<b>F828</b>	<b>F829</b>	<b>F830</b>	<b>F831</b>	<b>F832</b>	<b>F833</b>	<b>F834</b>	<b>F835</b>	<b>F836</b>	<b>F837</b>	<b>F838</b>	<b>F839</b>	<b>F840</b>	<b>F841</b>	<b>F842</b>	<b>F843</b>	<b>F844</b>	<b>F845</b>	<b>F846</b>	<b>F847</b>	<b>F848</b>	<b>F849</b>	<b>F850</b>	<b>F851</b>	<b>F852</b>	<b>F853</b>	<b>F854</b>	<b>F855</b>	<b>F856</b>	<b>F857</b>	<b>F858</b>	<b>F859</b>	<b>F860</b>	<b>F861</b>	<b>F862</b>	<b>F863</b>	<b>F864</b>	<b>F865</b>	<b>F866</b>	<b>F867</b>	<b>F868</b>	<b>F869</b>	<b>F870</b>	<b>F871</b>	<b>F872</b>	<b>F873</b>	<b>F874</b>	<b>F875</b>	<b>F876</b>	<b>F877</b>	<b>F878</b>	<b>F879</b>	<b>F880</b>	<b>F881</b>	<b>F882</b>	<b>F883</b>	<b>F884</b>	<b>F885</b>	<b>F886</b>	<b>F887</b>	<b>F888</b>	<b>F889</b>	<b>F890</b>	<b>F891</b>	<b>F892</b>	<b>F893</b>	<b>F894</b>	<b>F895</b>	<b>F896</b>	<b>F897</b>	<b>F898</b>	<b>F899</b>	<b>F900</b>	<b>F901</b>	<b>F902</b>	<b>F903</b>	<b>F904</b>	<b>F905</b>	<b>F906</b>	<b>F907</b>	<b>F908</b>	<b>F909</b>	<b>F910</b>	<b>F911</b>	<b>F912</b>	<b>F913</b>	<b>F914</b>	<b>F915</b>	<b>F916</b>	<b>F917</b>	<b>F918</b>	<b>F919</b>	<b>F920</b>	<b>F921</b>	<b>F922</b>
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E640	E641	E642	D643	E644	E650	E651	E652	E653	E654	E655	E656	E657	E658	E659	E660	E661	E662	E663	E664	E665	E666	E667	E668	E669	E670	E671	E672	E673	E674	E675	E676	E677	E678	E679	E680	E681	E682	E683	E684	E685	E686	E687	E688	E689	E690	E691	E692	E693	E694	E695	E696	E697	E698	E699	E700	E701	E702	E703	E704	E705	E706	E707	E708	E709	E710	E711	E712	E713	E714	E715	E716	E717	E718	E719	E720	E721	E722	E723	E724	E725	E726	E727	E728	E729	E730	E731	E732	E733	E734	E735	E736	E737	E738	E739	E740	E741	E742	E743	E744	E745	E746	E747	E748	E749	E750	E751	E752	E753	E754	E755	E756	E757	E758	E759	E760	E761	E762	E763	E764	E765	E766	E767	E768	E769	E770	E771	E772	E773	E774	E775	E776	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826	E827	E828	E829	E830	E831	E832	E833	E834	E835	E836	E837	E838	E839	E840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889	E890	E891	E892	E893	E894	E895	E896	E897	E898	E899	E900	E901	E902	E903	E904	E905	E906	E907	E908	E909	E910	E911	E912	E913	E914	E915	E916	E917	E918	E919	E920	E921	E922	E923	E924	E925	E926	E927	E928	E929	E930	E931	E932	E933	E934	E935	E936	E937	E938	E939	E940	E941	E942	E943	E944	E945	E946	E947	E948	E949	E950	E951	E952	E953	E954	E955	E956	E957	E958	E959	E960	E961	E962	E963	E964	E965	E966	E967	E968	E969	E970	E971	E972	E973	E974	E975	E976	E977	E978	E979	E980	E981	E982	E983	E984	E985	E986	E987	E988	E989	E990	E991	E992	E993	E994	E995	E996	E997	E998	E999
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[illegible]

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

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	42268	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: PLM, CHS, CA, PX6, NAG

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	0.49	0/4031	0.62	2/5469 (0.0%)
1	B	0.49	0/4031	0.62	3/5469 (0.1%)
1	C	0.49	0/4031	0.62	3/5469 (0.1%)
1	D	0.49	0/4031	0.63	2/5469 (0.0%)
All	All	0.49	0/16124	0.62	10/21876 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	5
1	C	0	5
1	D	0	5
All	All	0	20

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	278	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	278	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	278	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	384	ALA	C-N-CA	5.16	134.60	121.70
1	C	384	ALA	C-N-CA	5.14	134.55	121.70
1	B	384	ALA	C-N-CA	5.13	134.53	121.70
1	D	384	ALA	C-N-CA	5.12	134.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	643	ASP	CB-CG-OD1	5.01	122.81	118.30
1	C	643	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	LEU	Peptide
1	A	354	ASP	Peptide
1	A	361	ARG	Peptide
1	A	578	ASN	Peptide
1	A	627	SER	Peptide
1	B	291	LEU	Peptide
1	B	354	ASP	Peptide
1	B	361	ARG	Peptide
1	B	578	ASN	Peptide
1	B	627	SER	Peptide
1	C	291	LEU	Peptide
1	C	354	ASP	Peptide
1	C	361	ARG	Peptide
1	C	578	ASN	Peptide
1	C	627	SER	Peptide
1	D	291	LEU	Peptide
1	D	354	ASP	Peptide
1	D	361	ARG	Peptide
1	D	578	ASN	Peptide
1	D	627	SER	Peptide

## 5.2 Too-close contacts [i](#)

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	3926	0	3880	489	0
1	B	3926	0	3880	496	0
1	C	3926	0	3880	476	0
1	D	3926	0	3880	490	0
2	A	56	0	51	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	56	0	51	10	0
2	C	56	0	51	10	0
2	D	56	0	51	16	0
3	A	30	0	40	3	0
3	B	30	0	40	4	0
3	C	30	0	40	5	0
3	D	30	0	40	4	0
4	A	40	0	56	3	0
4	B	40	0	56	6	0
4	C	40	0	56	4	0
4	D	40	0	56	4	0
5	A	54	0	93	9	0
5	B	54	0	93	8	0
5	C	54	0	93	9	0
5	D	54	0	93	6	0
6	A	2	0	0	0	0
All	All	16426	0	16480	1816	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 55.

All (1816) 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:A:606:ILE:CD1	1:D:573:LEU:HD11	1.21	1.66
1:A:606:ILE:HD11	1:D:573:LEU:CD1	1.26	1.63
1:A:573:LEU:CD1	1:B:606:ILE:HD11	1.17	1.62
1:C:573:LEU:HD11	1:D:606:ILE:CD1	1.18	1.58
1:B:573:LEU:CD1	1:C:606:ILE:HD11	1.15	1.57
1:A:573:LEU:HD11	1:B:606:ILE:CD1	1.16	1.56
1:B:573:LEU:HD11	1:C:606:ILE:CD1	1.13	1.55
1:C:573:LEU:CD1	1:D:606:ILE:HD11	1.22	1.53
1:B:573:LEU:CD1	1:C:606:ILE:CD1	1.81	1.34
1:C:573:LEU:CD1	1:D:606:ILE:CD1	1.87	1.34
1:A:573:LEU:CD1	1:B:606:ILE:CD1	1.83	1.28
1:A:606:ILE:CD1	1:D:573:LEU:CD1	1.91	1.23
1:A:309:ILE:HD11	1:A:315:LEU:N	1.52	1.22
1:B:309:ILE:HD11	1:B:315:LEU:N	1.54	1.20
1:B:309:ILE:HG12	1:B:313:ASN:O	1.42	1.18
1:A:294:LYS:HE2	1:A:310:PHE:H	1.10	1.14
1:A:309:ILE:HG12	1:A:313:ASN:O	1.46	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ARG:O	2:B:1002:NAG:H82	1.50	1.12
1:C:361:ARG:O	2:C:1002:NAG:H82	1.50	1.11
1:A:361:ARG:O	2:A:1002:NAG:H82	1.50	1.11
1:D:361:ARG:O	2:D:1002:NAG:H82	1.50	1.10
1:B:294:LYS:HE2	1:B:310:PHE:H	1.08	1.10
1:A:309:ILE:HD11	1:A:315:LEU:H	0.92	1.08
1:D:309:ILE:HD11	1:D:314:LEU:C	1.75	1.07
1:C:294:LYS:HE2	1:C:310:PHE:H	1.08	1.07
1:D:309:ILE:HD11	1:D:314:LEU:CA	1.83	1.06
1:D:294:LYS:HE2	1:D:310:PHE:H	1.19	1.06
1:B:309:ILE:HG13	1:B:314:LEU:N	1.71	1.05
1:B:309:ILE:HD11	1:B:315:LEU:H	0.90	1.04
1:B:309:ILE:HG13	1:B:313:ASN:C	1.78	1.04
1:D:309:ILE:CD1	1:D:314:LEU:CA	2.36	1.03
1:B:309:ILE:CG1	1:B:313:ASN:O	2.07	1.02
1:D:309:ILE:HD11	1:D:315:LEU:N	1.72	1.02
1:D:309:ILE:HD12	1:D:313:ASN:C	1.80	1.01
1:A:309:ILE:HG13	1:A:314:LEU:N	1.76	1.01
1:B:309:ILE:CG1	1:B:313:ASN:C	2.30	0.98
1:C:361:ARG:O	2:C:1002:NAG:C8	2.11	0.98
1:A:361:ARG:O	2:A:1002:NAG:C8	2.11	0.98
1:D:309:ILE:HD12	1:D:313:ASN:O	1.63	0.98
1:D:309:ILE:CD1	1:D:314:LEU:N	2.27	0.98
1:A:306:ARG:HG2	1:A:308:PHE:CE1	1.98	0.98
1:B:361:ARG:O	2:B:1002:NAG:C8	2.11	0.97
1:D:361:ARG:O	2:D:1002:NAG:C8	2.11	0.97
1:A:309:ILE:CG1	1:A:313:ASN:C	2.35	0.95
1:D:310:PHE:O	1:D:312:GLU:OE1	1.85	0.95
1:A:314:LEU:HB3	1:A:429:TYR:HD2	1.34	0.93
1:D:294:LYS:NZ	1:D:309:ILE:HA	1.84	0.93
1:A:384:ALA:HA	1:A:385:THR:HG22	1.50	0.92
1:C:384:ALA:HA	1:C:385:THR:HG22	1.50	0.92
1:D:384:ALA:HA	1:D:385:THR:HG22	1.50	0.92
1:D:314:LEU:HB3	1:D:429:TYR:HD2	1.34	0.92
1:B:384:ALA:HA	1:B:385:THR:HG22	1.50	0.92
1:C:314:LEU:HB3	1:C:429:TYR:HD2	1.34	0.91
1:A:309:ILE:CG1	1:A:313:ASN:O	2.18	0.90
1:B:314:LEU:HB3	1:B:429:TYR:HD2	1.34	0.89
1:A:309:ILE:HG13	1:A:313:ASN:C	1.90	0.89
1:B:309:ILE:CD1	1:B:315:LEU:H	1.84	0.89
1:D:310:PHE:O	1:D:312:GLU:CD	2.11	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ARG:HG2	1:B:308:PHE:CE1	2.09	0.88
1:B:309:ILE:CD1	1:B:315:LEU:N	2.35	0.88
1:A:241:MET:HG3	1:A:242:MET:HG2	1.56	0.87
1:A:309:ILE:CD1	1:A:315:LEU:N	2.36	0.87
1:D:241:MET:HG3	1:D:242:MET:HG2	1.56	0.86
1:A:466:VAL:H	1:A:470:ASP:HB2	1.40	0.86
1:A:573:LEU:CD1	1:B:606:ILE:HD13	2.02	0.86
1:B:577:ILE:CD1	1:C:602:ILE:HD11	2.06	0.86
1:B:466:VAL:H	1:B:470:ASP:HB2	1.40	0.86
1:A:573:LEU:HD13	1:B:606:ILE:HD11	1.56	0.85
1:C:466:VAL:H	1:C:470:ASP:HB2	1.40	0.85
1:A:573:LEU:HD13	1:B:606:ILE:CD1	2.06	0.85
1:B:241:MET:HG3	1:B:242:MET:HG2	1.56	0.84
1:C:241:MET:HG3	1:C:242:MET:HG2	1.56	0.84
1:D:294:LYS:HE2	1:D:310:PHE:N	1.91	0.84
1:D:309:ILE:CD1	1:D:313:ASN:C	2.46	0.84
1:D:398:THR:HB	2:D:1001:NAG:C6	2.08	0.84
1:B:573:LEU:HD12	1:C:606:ILE:CD1	2.05	0.84
1:C:396:SER:HB2	1:C:398:THR:HG22	1.60	0.83
1:D:309:ILE:HD11	1:D:314:LEU:HA	1.60	0.83
1:D:398:THR:HB	2:D:1001:NAG:H61	1.61	0.83
1:B:573:LEU:CD1	1:C:606:ILE:HD12	2.07	0.83
1:D:466:VAL:H	1:D:470:ASP:HB2	1.40	0.83
1:C:294:LYS:HE2	1:C:310:PHE:N	1.93	0.83
1:D:396:SER:HB2	1:D:398:THR:HG22	1.60	0.83
1:B:606:ILE:CG2	1:B:607:ILE:N	2.42	0.82
1:A:606:ILE:CG2	1:A:607:ILE:N	2.42	0.82
1:A:306:ARG:HG2	1:A:308:PHE:CZ	2.14	0.82
1:A:525:ASN:OD1	1:A:526:ILE:N	2.13	0.82
1:B:611:TYR:O	1:B:615:ALA:N	2.13	0.82
1:B:573:LEU:CD1	1:C:606:ILE:HD13	2.04	0.82
1:A:396:SER:HB2	1:A:398:THR:HG22	1.60	0.82
1:B:396:SER:HB2	1:B:398:THR:HG22	1.60	0.81
1:D:525:ASN:OD1	1:D:526:ILE:N	2.13	0.81
1:A:611:TYR:O	1:A:615:ALA:N	2.13	0.81
1:A:294:LYS:HE2	1:A:310:PHE:N	1.93	0.81
1:A:247:TYR:OH	1:B:624:ASP:HA	1.81	0.81
1:B:650:GLU:HA	1:B:658:PRO:HG3	1.62	0.81
1:B:525:ASN:OD1	1:B:526:ILE:N	2.13	0.81
1:D:323:GLN:NE2	1:D:416:ASP:OD1	2.14	0.81
1:B:294:LYS:HE2	1:B:310:PHE:N	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLN:NE2	1:A:416:ASP:OD1	2.14	0.80
1:C:323:GLN:NE2	1:C:416:ASP:OD1	2.14	0.80
1:B:577:ILE:HD13	1:C:602:ILE:HD11	1.63	0.80
1:C:606:ILE:CG2	1:C:607:ILE:N	2.42	0.80
1:D:606:ILE:CG2	1:D:607:ILE:N	2.42	0.80
1:C:525:ASN:OD1	1:C:526:ILE:N	2.13	0.80
1:B:573:LEU:HD13	1:C:606:ILE:CD1	2.08	0.80
1:B:306:ARG:HG2	1:B:308:PHE:CZ	2.16	0.80
1:A:577:ILE:CD1	1:B:602:ILE:HD11	2.11	0.80
1:A:573:LEU:HD12	1:B:606:ILE:CD1	2.09	0.80
1:A:650:GLU:HA	1:A:658:PRO:HG3	1.62	0.80
1:C:573:LEU:CD1	1:D:606:ILE:HD13	2.06	0.80
1:A:406:VAL:HG13	1:A:414:TRP:HE1	1.47	0.79
1:B:323:GLN:NE2	1:B:416:ASP:OD1	2.14	0.79
1:D:436:PHE:O	1:D:460:LEU:N	2.15	0.79
1:B:269:ASN:OD1	1:B:272:THR:N	2.16	0.79
1:D:611:TYR:O	1:D:615:ALA:N	2.13	0.79
1:B:406:VAL:HG13	1:B:414:TRP:HE1	1.47	0.79
1:B:436:PHE:O	1:B:460:LEU:N	2.15	0.79
1:D:650:GLU:HA	1:D:658:PRO:HG3	1.62	0.79
1:C:650:GLU:HA	1:C:658:PRO:HG3	1.62	0.79
1:C:611:TYR:O	1:C:615:ALA:N	2.13	0.78
1:A:269:ASN:OD1	1:A:272:THR:N	2.15	0.78
1:A:247:TYR:HH	1:B:624:ASP:HA	1.48	0.78
1:D:406:VAL:HG13	1:D:414:TRP:HE1	1.47	0.78
1:C:418:GLY:O	1:C:420:ARG:NH2	2.17	0.78
1:D:418:GLY:O	1:D:420:ARG:NH2	2.17	0.78
1:A:418:GLY:O	1:A:420:ARG:NH2	2.17	0.78
1:C:406:VAL:HG13	1:C:414:TRP:HE1	1.47	0.78
1:C:436:PHE:O	1:C:460:LEU:N	2.15	0.78
1:B:380:TRP:O	1:B:385:THR:N	2.17	0.77
1:A:436:PHE:O	1:A:460:LEU:N	2.15	0.77
1:A:677:LEU:HD23	1:A:680:ILE:HD12	1.67	0.77
1:B:327:ARG:HG3	1:B:330:SER:HB2	1.65	0.77
1:B:418:GLY:O	1:B:420:ARG:NH2	2.17	0.77
1:D:380:TRP:O	1:D:385:THR:N	2.17	0.77
1:B:606:ILE:HG22	1:B:607:ILE:H	1.50	0.77
1:B:247:TYR:OH	1:C:624:ASP:HA	1.85	0.77
1:A:608:PHE:O	1:A:636:GLN:NE2	2.18	0.77
1:C:327:ARG:HG3	1:C:330:SER:HB2	1.65	0.77
1:D:677:LEU:HD23	1:D:680:ILE:HD12	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:HG3	1:A:330:SER:HB2	1.64	0.77
1:A:554:TRP:O	1:A:558:PHE:N	2.14	0.77
1:C:606:ILE:HG22	1:C:607:ILE:H	1.50	0.77
1:C:573:LEU:HD13	1:D:606:ILE:CD1	2.11	0.77
1:C:554:TRP:O	1:C:558:PHE:N	2.14	0.77
1:C:577:ILE:CD1	1:D:602:ILE:HD11	2.15	0.77
1:D:327:ARG:HG3	1:D:330:SER:HB2	1.65	0.77
1:B:608:PHE:O	1:B:636:GLN:NE2	2.18	0.76
1:B:577:ILE:CD1	1:C:602:ILE:CD1	2.62	0.76
1:A:606:ILE:HG22	1:A:607:ILE:H	1.50	0.76
1:A:606:ILE:HD13	1:D:573:LEU:CD1	2.10	0.76
1:B:677:LEU:HD23	1:B:680:ILE:HD12	1.67	0.76
1:C:247:TYR:OH	1:D:624:ASP:HA	1.85	0.76
1:A:573:LEU:CD1	1:B:606:ILE:HD12	2.13	0.76
1:C:677:LEU:HD23	1:C:680:ILE:HD12	1.67	0.76
1:A:236:ILE:O	1:A:240:GLY:N	2.18	0.76
1:D:606:ILE:HG22	1:D:607:ILE:H	1.50	0.76
1:C:653:ASN:HB2	1:C:656:LEU:HB3	1.69	0.75
1:C:236:ILE:O	1:C:240:GLY:N	2.17	0.75
1:B:681:ASN:HB2	1:C:674:ASN:HD21	1.51	0.75
1:D:236:ILE:O	1:D:240:GLY:N	2.18	0.75
1:B:653:ASN:HB2	1:B:656:LEU:HB3	1.69	0.75
1:A:498:HIS:HB3	1:A:501:HIS:HB3	1.69	0.75
1:D:653:ASN:HB2	1:D:656:LEU:HB3	1.69	0.75
1:A:653:ASN:HB2	1:A:656:LEU:HB3	1.68	0.75
1:A:380:TRP:O	1:A:385:THR:N	2.17	0.75
1:A:602:ILE:HD11	1:D:577:ILE:CD1	2.17	0.75
1:C:356:ALA:O	1:C:391:TYR:OH	2.04	0.75
1:D:309:ILE:CD1	1:D:314:LEU:HA	2.13	0.75
1:D:440:ARG:HB3	1:D:456:GLN:HB3	1.69	0.75
1:D:498:HIS:HB3	1:D:501:HIS:HB3	1.69	0.75
1:B:554:TRP:O	1:B:558:PHE:N	2.14	0.75
1:B:665:VAL:O	1:B:669:PHE:HB3	1.87	0.75
1:B:356:ALA:O	1:B:391:TYR:OH	2.04	0.74
1:A:573:LEU:HD11	1:B:606:ILE:HD13	1.55	0.74
1:A:440:ARG:HB3	1:A:456:GLN:HB3	1.69	0.74
1:B:309:ILE:HG13	1:B:314:LEU:CA	2.17	0.74
1:C:425:ASP:OD1	1:C:441:LEU:N	2.15	0.74
1:B:221:LEU:HA	1:B:224:LEU:HB2	1.69	0.74
1:C:380:TRP:O	1:C:385:THR:N	2.17	0.74
1:C:573:LEU:HD11	1:D:606:ILE:HD13	1.56	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:LEU:HA	1:D:224:LEU:HB2	1.69	0.74
1:A:356:ALA:O	1:A:391:TYR:OH	2.04	0.74
1:D:269:ASN:OD1	1:D:272:THR:N	2.15	0.74
1:D:356:ALA:O	1:D:391:TYR:OH	2.04	0.74
1:D:409:LEU:HB3	1:D:414:TRP:CD1	2.22	0.74
1:C:409:LEU:HB3	1:C:414:TRP:CD1	2.22	0.74
1:C:608:PHE:O	1:C:636:GLN:NE2	2.18	0.74
1:C:498:HIS:HB3	1:C:501:HIS:HB3	1.69	0.74
1:B:409:LEU:HB3	1:B:414:TRP:CD1	2.22	0.74
1:C:405:GLN:O	1:C:409:LEU:N	2.21	0.74
1:C:665:VAL:O	1:C:669:PHE:HB3	1.87	0.74
1:A:550:HIS:CE1	1:A:554:TRP:HE1	2.06	0.73
1:B:568:PHE:HA	1:B:571:ILE:HG12	1.70	0.73
1:C:269:ASN:OD1	1:C:272:THR:N	2.15	0.73
1:A:409:LEU:HB3	1:A:414:TRP:CD1	2.22	0.73
1:B:405:GLN:O	1:B:409:LEU:N	2.21	0.73
1:A:306:ARG:CG	1:A:308:PHE:CE1	2.70	0.73
1:B:498:HIS:HB3	1:B:501:HIS:HB3	1.69	0.73
1:A:624:ASP:HA	1:D:247:TYR:OH	1.88	0.73
1:A:577:ILE:HD13	1:B:602:ILE:HD11	1.70	0.73
1:A:665:VAL:O	1:A:669:PHE:HB3	1.87	0.73
1:B:425:ASP:OD1	1:B:441:LEU:N	2.15	0.73
1:B:440:ARG:HB3	1:B:456:GLN:HB3	1.69	0.73
1:C:409:LEU:O	1:C:414:TRP:N	2.19	0.73
1:D:608:PHE:O	1:D:636:GLN:NE2	2.18	0.73
1:A:405:GLN:O	1:A:409:LEU:N	2.21	0.73
1:D:554:TRP:O	1:D:558:PHE:N	2.14	0.73
1:A:444:GLU:HB2	1:A:452:ILE:HG23	1.71	0.73
1:C:550:HIS:CE1	1:C:554:TRP:HE1	2.07	0.73
1:D:550:HIS:CE1	1:D:554:TRP:HE1	2.07	0.73
1:A:221:LEU:HA	1:A:224:LEU:HB2	1.69	0.73
1:A:568:PHE:HA	1:A:571:ILE:HG12	1.70	0.73
1:B:248:TYR:O	1:B:252:MET:HG2	1.89	0.73
1:C:221:LEU:HA	1:C:224:LEU:HB2	1.69	0.73
1:C:440:ARG:HB3	1:C:456:GLN:HB3	1.69	0.73
1:D:360:PRO:O	1:D:366:TRP:NE1	2.22	0.73
1:A:248:TYR:O	1:A:252:MET:HG2	1.89	0.72
1:A:687:VAL:O	1:A:691:LEU:N	2.22	0.72
1:C:360:PRO:O	1:C:366:TRP:NE1	2.21	0.72
1:A:502:TYR:O	1:A:508:ASN:ND2	2.22	0.72
1:D:405:GLN:O	1:D:409:LEU:N	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:LEU:O	1:D:414:TRP:N	2.19	0.72
1:D:665:VAL:O	1:D:669:PHE:HB3	1.87	0.72
1:B:502:TYR:O	1:B:508:ASN:ND2	2.22	0.72
1:C:430:ASN:HD21	1:C:435:LEU:HB3	1.55	0.72
1:D:568:PHE:HA	1:D:571:ILE:HG12	1.71	0.72
1:C:444:GLU:HB2	1:C:452:ILE:HG23	1.71	0.72
1:D:348:TYR:HB2	1:D:420:ARG:HG3	1.71	0.72
1:D:444:GLU:HB2	1:D:452:ILE:HG23	1.71	0.72
1:A:657:GLY:O	1:A:660:TYR:N	2.23	0.72
1:D:687:VAL:O	1:D:691:LEU:N	2.22	0.72
1:B:236:ILE:O	1:B:240:GLY:N	2.18	0.72
1:B:430:ASN:HD21	1:B:435:LEU:HB3	1.55	0.72
1:C:606:ILE:O	1:C:610:ALA:N	2.21	0.72
1:D:502:TYR:O	1:D:508:ASN:ND2	2.22	0.72
1:B:550:HIS:CE1	1:B:554:TRP:HE1	2.07	0.72
1:B:657:GLY:O	1:B:660:TYR:N	2.23	0.72
1:C:348:TYR:HB2	1:C:420:ARG:HG3	1.71	0.72
1:C:687:VAL:O	1:C:691:LEU:N	2.22	0.72
1:C:573:LEU:HD12	1:D:606:ILE:CD1	2.14	0.72
1:C:502:TYR:O	1:C:508:ASN:ND2	2.22	0.71
1:C:573:LEU:CD1	1:D:606:ILE:HD12	2.15	0.71
1:D:604:PHE:O	1:D:608:PHE:N	2.19	0.71
1:C:687:VAL:HA	1:C:690:ASP:HB3	1.72	0.71
1:B:444:GLU:HB2	1:B:452:ILE:HG23	1.71	0.71
1:D:248:TYR:O	1:D:252:MET:HG2	1.89	0.71
1:D:309:ILE:HD13	1:D:314:LEU:N	2.05	0.71
1:C:248:TYR:O	1:C:252:MET:HG2	1.89	0.71
1:D:310:PHE:HB2	1:D:312:GLU:OE1	1.90	0.71
1:D:309:ILE:CD1	1:D:314:LEU:C	2.53	0.71
1:C:577:ILE:HD13	1:D:602:ILE:HD11	1.72	0.71
1:A:360:PRO:O	1:A:366:TRP:NE1	2.22	0.71
1:A:348:TYR:HB2	1:A:420:ARG:HG3	1.71	0.71
1:C:309:ILE:HD11	1:C:315:LEU:N	2.05	0.71
1:C:657:GLY:O	1:C:660:TYR:N	2.23	0.71
1:A:606:ILE:HD12	1:D:573:LEU:CD1	2.17	0.71
1:A:430:ASN:HD21	1:A:435:LEU:HB3	1.55	0.71
1:B:687:VAL:O	1:B:691:LEU:N	2.22	0.71
1:C:604:PHE:O	1:C:608:PHE:N	2.19	0.71
1:A:409:LEU:O	1:A:414:TRP:N	2.19	0.71
1:A:606:ILE:CD1	1:D:573:LEU:HD13	2.16	0.71
1:B:348:TYR:HB2	1:B:420:ARG:HG3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ARG:HG2	1:C:308:PHE:CE1	2.26	0.71
1:B:577:ILE:HD11	1:C:602:ILE:CD1	2.21	0.71
1:A:566:VAL:O	1:A:570:TRP:N	2.22	0.70
1:D:294:LYS:HZ3	1:D:309:ILE:HA	1.54	0.70
1:C:568:PHE:HA	1:C:571:ILE:HG12	1.71	0.70
1:D:687:VAL:HA	1:D:690:ASP:HB3	1.72	0.70
1:C:566:VAL:O	1:C:570:TRP:N	2.22	0.70
1:D:309:ILE:HD11	1:D:315:LEU:H	1.56	0.70
1:A:309:ILE:CD1	1:A:315:LEU:H	1.87	0.70
1:D:430:ASN:HD21	1:D:435:LEU:HB3	1.55	0.70
1:D:606:ILE:O	1:D:610:ALA:N	2.21	0.70
1:D:657:GLY:O	1:D:660:TYR:N	2.23	0.70
1:A:606:ILE:O	1:A:610:ALA:N	2.21	0.70
1:B:360:PRO:O	1:B:366:TRP:NE1	2.22	0.70
1:A:577:ILE:CD1	1:B:602:ILE:CD1	2.70	0.70
1:B:606:ILE:O	1:B:610:ALA:N	2.21	0.70
1:B:687:VAL:HA	1:B:690:ASP:HB3	1.72	0.70
1:C:232:ILE:HG22	1:C:236:ILE:HG13	1.74	0.70
1:A:606:ILE:CD1	1:D:573:LEU:HD12	2.16	0.70
1:A:357:PRO:O	1:A:361:ARG:NE	2.25	0.69
1:A:406:VAL:HA	1:A:409:LEU:HB2	1.74	0.69
1:A:681:ASN:HB2	1:B:674:ASN:HD21	1.55	0.69
1:A:328:ASN:OD1	1:A:329:GLY:N	2.26	0.69
1:A:562:ALA:O	1:A:565:THR:OG1	2.10	0.69
1:A:602:ILE:HD11	1:D:577:ILE:HD13	1.74	0.69
1:A:687:VAL:HA	1:A:690:ASP:HB3	1.72	0.69
1:D:404:ALA:O	1:D:408:SER:N	2.20	0.69
1:B:409:LEU:O	1:B:414:TRP:N	2.19	0.69
1:D:232:ILE:HG22	1:D:236:ILE:HG13	1.74	0.69
1:A:353:GLU:O	1:A:355:ARG:NH1	2.26	0.69
1:B:406:VAL:HA	1:B:409:LEU:HB2	1.74	0.69
1:D:328:ASN:OD1	1:D:329:GLY:N	2.26	0.69
1:B:357:PRO:O	1:B:361:ARG:NE	2.25	0.69
1:B:562:ALA:O	1:B:565:THR:OG1	2.10	0.69
1:C:353:GLU:O	1:C:355:ARG:NH1	2.26	0.69
1:A:309:ILE:CG1	1:A:314:LEU:N	2.54	0.69
1:D:353:GLU:O	1:D:355:ARG:NH1	2.26	0.69
1:B:328:ASN:OD1	1:B:329:GLY:N	2.26	0.69
1:A:448:THR:OG1	1:D:252:MET:SD	2.45	0.69
1:C:324:LEU:HD11	1:C:386:TYR:CE1	2.28	0.69
1:C:681:ASN:HB2	1:D:674:ASN:HD21	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ARG:HG2	1:B:323:GLN:H	1.58	0.68
1:B:690:ASP:OD1	1:B:693:GLN:NE2	2.27	0.68
1:C:406:VAL:HA	1:C:409:LEU:HB2	1.74	0.68
1:B:232:ILE:HG22	1:B:236:ILE:HG13	1.74	0.68
1:B:566:VAL:O	1:B:570:TRP:N	2.22	0.68
1:B:353:GLU:O	1:B:355:ARG:NH1	2.26	0.68
1:C:328:ASN:OD1	1:C:329:GLY:N	2.26	0.68
1:C:690:ASP:OD1	1:C:693:GLN:NE2	2.27	0.68
1:B:324:LEU:HD11	1:B:386:TYR:CE1	2.28	0.68
1:B:580:ASN:OD1	1:B:581:ARG:N	2.27	0.68
1:C:357:PRO:O	1:C:361:ARG:NE	2.25	0.68
1:D:357:PRO:O	1:D:361:ARG:NE	2.25	0.68
1:A:580:ASN:OD1	1:A:581:ARG:N	2.27	0.68
1:C:322:ARG:HG2	1:C:323:GLN:H	1.59	0.68
1:A:663:THR:HG21	5:D:1008:PLM:HG3	1.76	0.68
1:D:325:ARG:HH21	1:D:355:ARG:HA	1.59	0.68
1:D:562:ALA:O	1:D:565:THR:OG1	2.10	0.68
1:A:232:ILE:HG22	1:A:236:ILE:HG13	1.74	0.68
1:A:318:VAL:HG22	1:A:395:LEU:HB3	1.76	0.68
1:A:324:LEU:HD11	1:A:386:TYR:CE1	2.28	0.68
1:C:318:VAL:HG22	1:C:395:LEU:HB3	1.76	0.68
1:C:562:ALA:O	1:C:565:THR:OG1	2.11	0.68
1:A:349:SER:H	1:A:352:SER:HB3	1.59	0.68
1:B:604:PHE:O	1:B:608:PHE:N	2.18	0.68
1:D:324:LEU:HD11	1:D:386:TYR:CE1	2.28	0.68
1:D:406:VAL:HA	1:D:409:LEU:HB2	1.74	0.68
1:A:627:SER:N	1:A:632:CYS:SG	2.61	0.68
1:C:349:SER:H	1:C:352:SER:HB3	1.59	0.68
1:A:682:ASP:OD1	1:A:683:THR:N	2.25	0.68
1:B:309:ILE:CG1	1:B:314:LEU:CA	2.71	0.68
1:A:294:LYS:HD3	1:A:308:PHE:O	1.94	0.67
1:B:325:ARG:HH21	1:B:355:ARG:HA	1.59	0.67
3:C:1005:CHS:HZ2	3:C:1006:CHS:HE22	1.76	0.67
1:D:627:SER:N	1:D:632:CYS:SG	2.61	0.67
1:A:292:TYR:HD2	1:A:294:LYS:HE3	1.60	0.67
1:C:626:PHE:HD1	1:C:632:CYS:HG	1.41	0.67
1:D:690:ASP:OD1	1:D:693:GLN:NE2	2.26	0.67
1:B:223:GLU:O	1:B:226:THR:OG1	2.08	0.67
1:D:653:ASN:O	1:D:656:LEU:N	2.28	0.67
1:B:292:TYR:HD2	1:B:294:LYS:HE3	1.59	0.67
1:D:318:VAL:HG22	1:D:395:LEU:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ILE:HG13	1:A:314:LEU:CA	2.24	0.67
1:B:404:ALA:O	1:B:408:SER:N	2.20	0.67
5:B:1008:PLM:HG3	1:C:663:THR:HG21	1.77	0.67
1:D:398:THR:HA	2:D:1001:NAG:O6	1.95	0.67
1:A:674:ASN:HD21	1:D:681:ASN:HB2	1.58	0.67
1:C:325:ARG:HH21	1:C:355:ARG:HA	1.59	0.67
1:D:349:SER:H	1:D:352:SER:HB3	1.59	0.67
1:D:580:ASN:OD1	1:D:581:ARG:N	2.27	0.67
1:B:237:LEU:O	1:B:241:MET:N	2.21	0.67
1:B:309:ILE:CG1	1:B:314:LEU:HA	2.24	0.67
1:B:318:VAL:HG22	1:B:395:LEU:HB3	1.76	0.67
1:A:577:ILE:HD11	1:B:602:ILE:CD1	2.25	0.67
1:A:322:ARG:HG2	1:A:323:GLN:H	1.59	0.67
1:A:417:ARG:NH1	1:D:311:TYR:O	2.28	0.67
1:C:580:ASN:OD1	1:C:581:ARG:N	2.27	0.67
1:C:577:ILE:CD1	1:D:602:ILE:CD1	2.72	0.67
1:A:626:PHE:HD1	1:A:632:CYS:HG	1.40	0.67
1:B:349:SER:H	1:B:352:SER:HB3	1.59	0.67
3:B:1005:CHS:HZ2	3:B:1006:CHS:HE22	1.77	0.66
1:B:682:ASP:OD1	1:B:683:THR:N	2.26	0.66
1:C:682:ASP:OD1	1:C:683:THR:N	2.26	0.66
1:A:690:ASP:OD1	1:A:693:GLN:NE2	2.27	0.66
1:D:292:TYR:HD2	1:D:294:LYS:HE3	1.59	0.66
1:D:427:SER:OG	1:D:437:CYS:O	2.10	0.66
1:A:604:PHE:O	1:A:608:PHE:N	2.19	0.66
1:C:223:GLU:O	1:C:226:THR:OG1	2.08	0.66
1:B:653:ASN:O	1:B:656:LEU:N	2.28	0.66
1:C:292:TYR:HD2	1:C:294:LYS:HE3	1.60	0.66
1:C:653:ASN:O	1:C:656:LEU:N	2.28	0.66
1:A:325:ARG:HH21	1:A:355:ARG:HA	1.59	0.66
1:D:223:GLU:O	1:D:226:THR:OG1	2.08	0.66
1:D:322:ARG:HG2	1:D:323:GLN:H	1.58	0.66
1:C:237:LEU:O	1:C:241:MET:N	2.21	0.66
1:A:653:ASN:O	1:A:656:LEU:N	2.28	0.66
1:A:425:ASP:OD1	1:A:441:LEU:N	2.15	0.66
1:B:427:SER:OG	1:B:437:CYS:O	2.10	0.66
1:C:252:MET:SD	1:D:448:THR:OG1	2.49	0.66
3:A:1005:CHS:HZ2	3:A:1006:CHS:HE22	1.77	0.65
1:A:427:SER:OG	1:A:437:CYS:O	2.10	0.65
1:C:247:TYR:HH	1:D:624:ASP:HA	1.59	0.65
1:B:398:THR:HG23	1:B:398:THR:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:ARG:CG	1:B:308:PHE:CE1	2.78	0.65
1:A:602:ILE:CD1	1:D:577:ILE:CD1	2.74	0.65
1:A:404:ALA:O	1:A:408:SER:N	2.20	0.65
1:B:309:ILE:CG1	1:B:314:LEU:N	2.54	0.65
1:A:309:ILE:CG1	1:A:314:LEU:CA	2.74	0.65
1:C:398:THR:O	1:C:398:THR:HG23	1.96	0.65
1:C:547:ASN:OD1	1:C:549:GLU:N	2.29	0.65
1:D:425:ASP:OD1	1:D:441:LEU:N	2.15	0.65
1:A:682:ASP:O	1:A:686:GLU:N	2.30	0.65
1:B:362:ASN:OD1	2:B:1002:NAG:C7	2.44	0.65
1:C:362:ASN:OD1	2:C:1002:NAG:C7	2.44	0.65
1:C:404:ALA:O	1:C:408:SER:N	2.20	0.65
1:D:606:ILE:HG23	1:D:607:ILE:N	2.12	0.65
1:B:547:ASN:OD1	1:B:549:GLU:N	2.29	0.65
1:D:682:ASP:OD1	1:D:683:THR:N	2.26	0.65
1:A:362:ASN:OD1	2:A:1002:NAG:C7	2.44	0.65
1:A:547:ASN:OD1	1:A:549:GLU:N	2.29	0.64
1:D:547:ASN:OD1	1:D:549:GLU:N	2.29	0.64
1:A:398:THR:O	1:A:398:THR:HG23	1.96	0.64
1:C:606:ILE:HG23	1:C:607:ILE:N	2.12	0.64
1:C:682:ASP:O	1:C:686:GLU:N	2.30	0.64
1:A:502:TYR:HD1	1:A:508:ASN:HD22	1.46	0.64
1:B:502:TYR:HD1	1:B:508:ASN:HD22	1.46	0.64
1:D:502:TYR:HD1	1:D:508:ASN:HD22	1.46	0.64
1:A:232:ILE:O	1:A:236:ILE:N	2.24	0.64
1:D:362:ASN:OD1	2:D:1002:NAG:C7	2.44	0.64
1:C:241:MET:HB2	1:C:461:LYS:HD3	1.80	0.64
1:A:606:ILE:HG23	1:A:607:ILE:N	2.12	0.64
1:C:436:PHE:N	1:C:460:LEU:O	2.29	0.64
1:C:502:TYR:HD1	1:C:508:ASN:HD22	1.46	0.64
1:D:398:THR:HG23	1:D:398:THR:O	1.96	0.64
1:A:467:THR:OG1	1:B:335:GLN:OE1	2.15	0.64
1:C:427:SER:OG	1:C:437:CYS:O	2.10	0.64
1:A:223:GLU:O	1:A:226:THR:OG1	2.08	0.63
3:D:1005:CHS:HZ2	3:D:1006:CHS:HE22	1.79	0.63
1:A:384:ALA:HA	1:A:385:THR:CG2	2.27	0.63
1:B:458:GLN:NE2	1:B:459:PRO:HD2	2.14	0.63
1:B:241:MET:HB2	1:B:461:LYS:HD3	1.80	0.63
1:B:661:PHE:O	1:B:665:VAL:HG12	1.99	0.63
1:C:577:ILE:HD11	1:D:602:ILE:CD1	2.28	0.63
1:C:661:PHE:O	1:C:665:VAL:HG12	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:MET:HB2	1:D:461:LYS:HD3	1.80	0.63
1:A:458:GLN:NE2	1:A:459:PRO:HD2	2.14	0.63
1:B:606:ILE:HG23	1:B:607:ILE:N	2.12	0.63
1:C:555:GLN:O	1:C:559:ASN:N	2.24	0.63
1:D:458:GLN:NE2	1:D:459:PRO:HD2	2.14	0.63
1:D:540:GLU:HA	1:D:546:PRO:HD3	1.80	0.63
1:A:540:GLU:HA	1:A:546:PRO:HD3	1.80	0.63
1:B:677:LEU:HD21	1:C:673:LEU:HD12	1.80	0.63
1:A:555:GLN:O	1:A:559:ASN:N	2.24	0.63
1:D:661:PHE:O	1:D:665:VAL:HG12	1.99	0.63
1:C:309:ILE:O	1:C:312:GLU:N	2.29	0.63
1:C:311:TYR:O	1:D:417:ARG:NH1	2.31	0.63
1:B:502:TYR:HB2	1:B:508:ASN:HB3	1.81	0.63
1:C:540:GLU:HA	1:C:546:PRO:HD3	1.80	0.62
1:A:361:ARG:O	2:A:1002:NAG:H81	1.99	0.62
1:B:311:TYR:O	1:C:417:ARG:NH1	2.32	0.62
1:A:241:MET:HB2	1:A:461:LYS:HD3	1.80	0.62
1:A:655:VAL:HG11	4:D:1007:PX6:H41	1.82	0.62
1:C:458:GLN:NE2	1:C:459:PRO:HD2	2.14	0.62
1:D:384:ALA:HA	1:D:385:THR:CG2	2.27	0.62
1:D:502:TYR:HB2	1:D:508:ASN:HB3	1.82	0.62
1:B:232:ILE:O	1:B:236:ILE:N	2.24	0.62
1:B:476:CYS:HA	1:B:479:ILE:HD12	1.82	0.62
1:D:566:VAL:O	1:D:570:TRP:N	2.22	0.62
1:A:502:TYR:HB2	1:A:508:ASN:HB3	1.81	0.62
1:B:509:CYS:O	1:B:513:VAL:N	2.33	0.62
1:B:540:GLU:HA	1:B:546:PRO:HD3	1.80	0.62
1:C:323:GLN:HG2	1:C:324:LEU:N	2.15	0.62
1:D:294:LYS:CE	1:D:310:PHE:H	2.03	0.62
1:D:436:PHE:N	1:D:460:LEU:O	2.29	0.62
1:A:683:THR:HA	1:A:686:GLU:HB3	1.82	0.62
1:B:361:ARG:O	2:B:1002:NAG:H81	1.99	0.62
1:B:681:ASN:HB2	1:C:674:ASN:ND2	2.12	0.62
1:C:398:THR:OG1	1:C:400:GLU:OE1	2.16	0.62
1:C:502:TYR:HB2	1:C:508:ASN:HB3	1.82	0.62
1:D:323:GLN:HG2	1:D:324:LEU:N	2.15	0.62
1:D:509:CYS:O	1:D:513:VAL:N	2.33	0.62
1:A:466:VAL:HG12	1:A:468:THR:H	1.65	0.62
1:A:661:PHE:O	1:A:665:VAL:HG12	1.99	0.62
1:B:683:THR:HA	1:B:686:GLU:HB3	1.82	0.62
1:C:683:THR:HA	1:C:686:GLU:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:ARG:O	2:D:1002:NAG:H81	1.99	0.62
1:D:396:SER:CB	1:D:398:THR:HG22	2.30	0.62
1:B:317:GLY:HA3	1:B:545:PHE:HD1	1.65	0.62
1:D:223:GLU:CD	1:D:227:TYR:HE2	2.03	0.62
1:D:683:THR:HA	1:D:686:GLU:HB3	1.82	0.62
1:A:317:GLY:HA3	1:A:545:PHE:HD1	1.65	0.61
1:B:223:GLU:CD	1:B:227:TYR:HE2	2.04	0.61
1:C:476:CYS:HA	1:C:479:ILE:HD12	1.82	0.61
1:C:570:TRP:HE1	1:D:606:ILE:HG12	1.65	0.61
1:A:404:ALA:HA	1:A:407:ALA:HB3	1.83	0.61
1:B:682:ASP:O	1:B:686:GLU:N	2.30	0.61
1:A:223:GLU:CD	1:A:227:TYR:HE2	2.03	0.61
1:A:237:LEU:O	1:A:241:MET:N	2.21	0.61
1:A:476:CYS:HA	1:A:479:ILE:HD12	1.82	0.61
1:B:247:TYR:HH	1:C:624:ASP:HA	1.63	0.61
1:B:323:GLN:HG2	1:B:324:LEU:N	2.15	0.61
1:C:317:GLY:HA3	1:C:545:PHE:HD1	1.65	0.61
1:C:404:ALA:HA	1:C:407:ALA:HB3	1.83	0.61
1:A:509:CYS:O	1:A:513:VAL:N	2.33	0.61
1:B:404:ALA:HA	1:B:407:ALA:HB3	1.83	0.61
1:C:254:SER:OG	1:C:255:GLN:N	2.33	0.61
1:B:384:ALA:HA	1:B:385:THR:CG2	2.27	0.61
1:B:555:GLN:O	1:B:559:ASN:N	2.24	0.61
5:A:1008:PLM:HG3	1:B:663:THR:HG21	1.83	0.61
1:D:682:ASP:O	1:D:686:GLU:N	2.30	0.61
1:A:323:GLN:HG2	1:A:324:LEU:N	2.15	0.61
1:B:352:SER:N	1:B:353:GLU:OE1	2.34	0.61
1:B:577:ILE:HG12	1:C:602:ILE:HD13	1.83	0.61
1:B:268:THR:OG1	1:B:272:THR:O	2.19	0.61
1:B:466:VAL:HG12	1:B:468:THR:H	1.65	0.61
1:C:466:VAL:HG12	1:C:468:THR:H	1.65	0.61
1:A:268:THR:OG1	1:A:272:THR:O	2.19	0.61
1:B:254:SER:OG	1:B:255:GLN:N	2.33	0.61
1:C:361:ARG:O	2:C:1002:NAG:H81	1.99	0.61
1:C:684:TYR:O	1:C:687:VAL:HG22	2.01	0.61
1:D:404:ALA:HA	1:D:407:ALA:HB3	1.83	0.61
5:C:1008:PLM:HG3	1:D:663:THR:HG21	1.83	0.61
1:B:573:LEU:HD11	1:C:606:ILE:HD13	1.57	0.61
1:C:223:GLU:CD	1:C:227:TYR:HE2	2.04	0.61
1:C:352:SER:N	1:C:353:GLU:OE1	2.34	0.61
1:C:509:CYS:O	1:C:513:VAL:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:517:LEU:HB3	1:C:565:THR:HG22	1.83	0.60
1:D:466:VAL:HG12	1:D:468:THR:H	1.65	0.60
1:A:602:ILE:CD1	1:D:577:ILE:HD11	2.31	0.60
1:A:684:TYR:O	1:A:687:VAL:HG22	2.01	0.60
1:B:589:THR:HA	1:B:592:ARG:HB3	1.83	0.60
1:D:352:SER:N	1:D:353:GLU:OE1	2.34	0.60
1:A:589:THR:HA	1:A:592:ARG:HB3	1.83	0.60
1:C:384:ALA:HA	1:C:385:THR:CG2	2.27	0.60
1:C:502:TYR:HB2	1:C:508:ASN:CB	2.32	0.60
1:A:254:SER:OG	1:A:255:GLN:N	2.33	0.60
1:A:570:TRP:HE1	1:B:606:ILE:HG12	1.65	0.60
1:D:268:THR:OG1	1:D:272:THR:O	2.19	0.60
1:D:476:CYS:HA	1:D:479:ILE:HD12	1.82	0.60
1:D:502:TYR:HB2	1:D:508:ASN:CB	2.31	0.60
1:D:684:TYR:O	1:D:687:VAL:HG22	2.01	0.60
1:A:262:VAL:N	1:A:268:THR:O	2.33	0.60
1:A:417:ARG:NH1	1:D:311:TYR:HB3	2.16	0.60
1:D:317:GLY:HA3	1:D:545:PHE:HD1	1.65	0.60
1:A:314:LEU:HB3	1:A:429:TYR:CD2	2.26	0.60
1:B:466:VAL:HB	1:B:470:ASP:N	2.17	0.60
1:C:466:VAL:HB	1:C:470:ASP:N	2.17	0.60
1:D:237:LEU:O	1:D:241:MET:N	2.21	0.60
1:D:517:LEU:HB3	1:D:565:THR:HG22	1.83	0.60
1:D:555:GLN:O	1:D:559:ASN:N	2.24	0.60
1:A:502:TYR:HB2	1:A:508:ASN:CB	2.31	0.60
1:B:221:LEU:O	1:B:225:VAL:N	2.29	0.60
1:B:684:TYR:O	1:B:687:VAL:HG22	2.01	0.60
1:A:396:SER:CB	1:A:398:THR:HG22	2.30	0.60
1:A:466:VAL:HB	1:A:470:ASP:N	2.17	0.60
1:A:352:SER:N	1:A:353:GLU:OE1	2.34	0.60
1:B:396:SER:CB	1:B:398:THR:HG22	2.30	0.60
1:D:466:VAL:HB	1:D:470:ASP:N	2.17	0.60
1:A:309:ILE:CG1	1:A:314:LEU:HA	2.31	0.60
1:B:502:TYR:HB2	1:B:508:ASN:CB	2.31	0.60
1:C:268:THR:OG1	1:C:272:THR:O	2.19	0.60
1:B:570:TRP:HE1	1:C:606:ILE:HG12	1.67	0.60
1:A:681:ASN:HB2	1:B:674:ASN:ND2	2.17	0.59
1:B:310:PHE:HB2	1:B:312:GLU:OE1	2.02	0.59
1:B:572:LYS:HG3	1:B:576:PHE:CE2	2.37	0.59
1:C:310:PHE:HB2	1:C:312:GLU:OE1	2.02	0.59
1:C:589:THR:HA	1:C:592:ARG:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:TRP:HE1	1:D:606:ILE:CG1	2.15	0.59
4:B:1007:PX6:H41	1:C:655:VAL:HG11	1.85	0.59
1:B:517:LEU:HB3	1:B:565:THR:HG22	1.83	0.59
1:A:221:LEU:O	1:A:225:VAL:N	2.29	0.59
1:A:463:ILE:HD12	1:A:465:TYR:HB2	1.84	0.59
1:C:572:LYS:HG3	1:C:576:PHE:CE2	2.37	0.59
1:C:627:SER:N	1:C:632:CYS:SG	2.61	0.59
1:D:589:THR:HA	1:D:592:ARG:HB3	1.83	0.59
1:B:570:TRP:HE1	1:C:606:ILE:CG1	2.15	0.59
1:B:627:SER:N	1:B:632:CYS:SG	2.61	0.59
1:C:262:VAL:N	1:C:268:THR:O	2.33	0.59
1:D:254:SER:OG	1:D:255:GLN:N	2.33	0.59
1:C:615:ALA:HA	1:C:619:PHE:HD2	1.68	0.59
1:A:572:LYS:HG3	1:A:576:PHE:CE2	2.37	0.59
1:B:314:LEU:HB3	1:B:429:TYR:CD2	2.26	0.59
1:B:436:PHE:N	1:B:460:LEU:O	2.29	0.59
1:B:674:ASN:O	1:B:677:LEU:N	2.36	0.59
1:C:309:ILE:HG13	1:C:314:LEU:CA	2.33	0.59
1:D:262:VAL:N	1:D:268:THR:O	2.33	0.59
1:D:466:VAL:N	1:D:470:ASP:HB2	2.16	0.59
1:D:572:LYS:HG3	1:D:576:PHE:CE2	2.37	0.59
1:A:436:PHE:N	1:A:460:LEU:O	2.29	0.59
1:A:674:ASN:O	1:A:677:LEU:N	2.36	0.59
1:B:463:ILE:HD12	1:B:465:TYR:HB2	1.84	0.59
1:D:615:ALA:HA	1:D:619:PHE:HD2	1.68	0.59
1:A:466:VAL:N	1:A:470:ASP:HB2	2.16	0.59
1:A:517:LEU:HB3	1:A:565:THR:HG22	1.83	0.59
1:C:307:SER:HB3	1:C:397:ARG:NH2	2.17	0.59
1:C:674:ASN:O	1:C:677:LEU:N	2.36	0.59
1:B:615:ALA:HA	1:B:619:PHE:HD2	1.68	0.59
1:C:681:ASN:HB2	1:D:674:ASN:ND2	2.18	0.59
1:A:310:PHE:HB2	1:A:312:GLU:OE1	2.02	0.58
1:C:396:SER:CB	1:C:398:THR:HG22	2.30	0.58
1:A:606:ILE:HG12	1:D:570:TRP:HE1	1.68	0.58
1:C:573:LEU:HD13	1:D:606:ILE:HD11	1.62	0.58
1:A:674:ASN:ND2	1:D:681:ASN:HB2	2.18	0.58
1:B:470:ASP:O	1:B:474:ALA:N	2.22	0.58
1:A:653:ASN:ND2	1:D:456:GLN:OE1	2.36	0.58
1:D:463:ILE:HD12	1:D:465:TYR:HB2	1.84	0.58
1:A:606:ILE:CG1	1:D:570:TRP:HE1	2.16	0.58
1:D:221:LEU:O	1:D:225:VAL:N	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:604:PHE:HA	1:D:607:ILE:HG22	1.85	0.58
1:A:615:ALA:HA	1:A:619:PHE:HD2	1.68	0.58
1:C:463:ILE:HD12	1:C:465:TYR:HB2	1.84	0.58
1:C:539:LEU:HD11	2:C:1004:NAG:O6	2.03	0.58
1:D:294:LYS:CE	1:D:309:ILE:HA	2.34	0.58
1:D:674:ASN:O	1:D:677:LEU:N	2.36	0.58
1:A:624:ASP:HA	1:D:247:TYR:HH	1.65	0.58
1:C:624:ASP:O	1:C:626:PHE:N	2.37	0.58
1:D:325:ARG:HH21	1:D:356:ALA:H	1.51	0.58
1:A:677:LEU:HD22	1:B:674:ASN:HB2	1.86	0.58
1:C:677:LEU:HD21	1:D:673:LEU:HD12	1.86	0.58
1:D:566:VAL:HA	1:D:569:VAL:HB	1.86	0.58
1:D:677:LEU:O	1:D:681:ASN:N	2.24	0.58
1:D:470:ASP:O	1:D:474:ALA:N	2.22	0.58
1:A:624:ASP:O	1:A:626:PHE:N	2.37	0.58
1:B:604:PHE:HA	1:B:607:ILE:HG22	1.85	0.58
1:D:539:LEU:HD11	2:D:1004:NAG:O6	2.03	0.58
1:A:673:LEU:HD12	1:D:677:LEU:HD21	1.86	0.58
1:A:263:SER:OG	1:A:285:GLY:O	2.22	0.58
1:B:624:ASP:O	1:B:626:PHE:N	2.37	0.58
1:C:232:ILE:O	1:C:236:ILE:N	2.24	0.58
1:B:573:LEU:HD13	1:C:606:ILE:HD11	1.60	0.58
1:A:306:ARG:CG	1:A:308:PHE:HE1	2.16	0.58
1:A:604:PHE:HA	1:A:607:ILE:HG22	1.85	0.58
1:B:263:SER:OG	1:B:285:GLY:O	2.22	0.58
1:A:570:TRP:HE1	1:B:606:ILE:CG1	2.17	0.58
1:A:456:GLN:OE1	1:B:653:ASN:ND2	2.35	0.58
1:C:325:ARG:HH21	1:C:356:ALA:H	1.51	0.58
1:A:224:LEU:HA	1:A:227:TYR:HD2	1.69	0.57
1:C:263:SER:OG	1:C:285:GLY:O	2.22	0.57
1:C:306:ARG:HG2	1:C:308:PHE:CZ	2.39	0.57
1:C:406:VAL:HA	1:C:409:LEU:HD12	1.86	0.57
1:D:224:LEU:HA	1:D:227:TYR:HD2	1.69	0.57
1:C:309:ILE:HG13	1:C:314:LEU:HA	1.86	0.57
1:D:263:SER:OG	1:D:285:GLY:O	2.22	0.57
1:A:674:ASN:HB2	1:D:677:LEU:HD22	1.86	0.57
1:A:322:ARG:HB3	1:A:423:PHE:HB2	1.87	0.57
1:A:566:VAL:HA	1:A:569:VAL:HB	1.86	0.57
1:C:224:LEU:HA	1:C:227:TYR:HD2	1.69	0.57
1:A:539:LEU:HD11	2:A:1004:NAG:O6	2.03	0.57
1:B:539:LEU:HD11	2:B:1004:NAG:O6	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:604:PHE:HA	1:C:607:ILE:HG22	1.85	0.57
1:D:624:ASP:O	1:D:626:PHE:N	2.37	0.57
1:A:325:ARG:HH21	1:A:356:ALA:H	1.51	0.57
1:A:432:ASN:ND2	1:B:447:ALA:O	2.37	0.57
1:C:221:LEU:O	1:C:225:VAL:N	2.29	0.57
1:C:677:LEU:HD22	1:D:674:ASN:HB2	1.87	0.57
1:A:311:TYR:O	1:B:417:ARG:NH1	2.38	0.57
1:B:406:VAL:HA	1:B:409:LEU:HD12	1.87	0.57
1:C:677:LEU:O	1:C:681:ASN:N	2.24	0.57
1:A:382:ILE:HG23	1:A:383:ILE:H	1.70	0.57
1:B:224:LEU:HA	1:B:227:TYR:HD2	1.69	0.57
1:A:677:LEU:HD21	1:B:673:LEU:HD12	1.87	0.57
1:B:382:ILE:HG23	1:B:383:ILE:H	1.70	0.57
1:B:533:GLU:HA	1:B:536:LEU:HD22	1.87	0.57
1:B:566:VAL:HA	1:B:569:VAL:HB	1.86	0.57
1:B:677:LEU:O	1:B:681:ASN:N	2.24	0.57
1:C:533:GLU:HA	1:C:536:LEU:HD22	1.87	0.57
1:B:640:ILE:HD12	1:B:672:LEU:HD21	1.87	0.56
1:C:466:VAL:N	1:C:470:ASP:HB2	2.16	0.56
1:C:566:VAL:HA	1:C:569:VAL:HB	1.86	0.56
1:A:395:LEU:HG	1:A:396:SER:H	1.70	0.56
1:D:322:ARG:HB3	1:D:423:PHE:HB2	1.87	0.56
1:D:406:VAL:HA	1:D:409:LEU:HD12	1.87	0.56
1:A:323:GLN:HG2	1:A:324:LEU:H	1.70	0.56
1:A:489:VAL:HA	1:A:492:ILE:HD12	1.87	0.56
1:B:489:VAL:HA	1:B:492:ILE:HD12	1.87	0.56
1:C:489:VAL:HA	1:C:492:ILE:HD12	1.87	0.56
1:C:323:GLN:HG2	1:C:324:LEU:H	1.70	0.56
1:C:640:ILE:HD12	1:C:672:LEU:HD21	1.87	0.56
1:D:398:THR:OG1	1:D:400:GLU:OE1	2.16	0.56
1:D:640:ILE:HD12	1:D:672:LEU:HD21	1.87	0.56
1:D:232:ILE:O	1:D:236:ILE:N	2.24	0.56
1:A:470:ASP:O	1:A:474:ALA:N	2.22	0.56
1:B:325:ARG:HH21	1:B:356:ALA:H	1.51	0.56
1:D:395:LEU:HG	1:D:396:SER:H	1.70	0.56
1:B:322:ARG:HB3	1:B:423:PHE:HB2	1.87	0.56
1:D:398:THR:CA	2:D:1001:NAG:O6	2.54	0.56
1:A:509:CYS:O	1:A:513:VAL:HG23	2.06	0.56
1:C:395:LEU:HG	1:C:396:SER:H	1.70	0.56
1:C:456:GLN:OE1	1:D:653:ASN:ND2	2.36	0.56
1:A:324:LEU:HD11	1:A:386:TYR:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:LEU:HB3	1:C:429:TYR:CD2	2.26	0.56
1:C:509:CYS:O	1:C:513:VAL:HG23	2.06	0.56
1:D:226:THR:HB	1:D:483:PHE:HZ	1.71	0.56
1:A:398:THR:OG1	1:A:400:GLU:OE1	2.16	0.56
1:A:401:GLU:O	1:A:405:GLN:N	2.27	0.56
1:B:323:GLN:HG2	1:B:324:LEU:H	1.70	0.56
1:C:226:THR:HB	1:C:483:PHE:HZ	1.71	0.56
1:D:323:GLN:HG2	1:D:324:LEU:H	1.70	0.56
3:A:1006:CHS:OH	3:A:1006:CHS:O	2.23	0.56
1:A:406:VAL:HA	1:A:409:LEU:HD12	1.87	0.56
1:A:533:GLU:HA	1:A:536:LEU:HD22	1.87	0.56
1:C:322:ARG:HB3	1:C:423:PHE:HB2	1.87	0.56
1:B:509:CYS:O	1:B:513:VAL:HG23	2.06	0.55
1:B:458:GLN:HG2	1:B:556:ILE:HG12	1.87	0.55
1:D:533:GLU:HA	1:D:536:LEU:HD22	1.87	0.55
1:D:458:GLN:HG2	1:D:556:ILE:HG12	1.87	0.55
1:C:382:ILE:HG23	1:C:383:ILE:H	1.70	0.55
1:D:489:VAL:HA	1:D:492:ILE:HD12	1.87	0.55
1:D:509:CYS:O	1:D:513:VAL:HG23	2.06	0.55
1:D:591:SER:HA	1:D:594:ALA:HB3	1.89	0.55
1:A:306:ARG:CG	1:A:308:PHE:CZ	2.88	0.55
1:B:262:VAL:N	1:B:268:THR:O	2.33	0.55
1:B:226:THR:HB	1:B:483:PHE:HZ	1.71	0.55
1:B:250:THR:OG1	1:B:251:ARG:N	2.40	0.55
1:D:382:ILE:HG23	1:D:383:ILE:H	1.70	0.55
1:A:640:ILE:HD12	1:A:672:LEU:HD21	1.87	0.55
1:C:432:ASN:ND2	1:D:447:ALA:O	2.38	0.55
1:A:528:ARG:HH22	1:A:550:HIS:HE1	1.55	0.55
1:A:677:LEU:O	1:A:681:ASN:N	2.24	0.55
1:A:688:LYS:O	1:A:692:ALA:N	2.39	0.55
1:C:324:LEU:HD11	1:C:386:TYR:CZ	2.41	0.55
1:D:324:LEU:HD11	1:D:386:TYR:CZ	2.41	0.55
1:A:250:THR:OG1	1:A:251:ARG:N	2.40	0.55
1:A:623:VAL:HG22	1:A:624:ASP:O	2.07	0.55
1:A:677:LEU:O	1:B:674:ASN:ND2	2.39	0.55
1:C:250:THR:OG1	1:C:251:ARG:N	2.40	0.55
1:A:458:GLN:HG2	1:A:556:ILE:HG12	1.87	0.55
1:C:528:ARG:HH22	1:C:550:HIS:HE1	1.55	0.55
1:C:668:MET:HA	1:C:671:ILE:HG22	1.89	0.55
1:C:688:LYS:O	1:C:692:ALA:N	2.39	0.55
1:A:641:LEU:HD21	1:B:642:GLY:HA2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:SER:HA	1:C:594:ALA:HB3	1.89	0.55
1:A:591:SER:HA	1:A:594:ALA:HB3	1.89	0.55
1:B:362:ASN:OD1	2:B:1002:NAG:N2	2.40	0.55
1:C:362:ASN:OD1	2:C:1002:NAG:N2	2.40	0.55
1:C:638:ARG:HE	1:C:643:ASP:CG	2.10	0.55
1:D:250:THR:OG1	1:D:251:ARG:N	2.40	0.55
1:A:362:ASN:OD1	2:A:1002:NAG:N2	2.40	0.54
1:B:528:ARG:HH22	1:B:550:HIS:HE1	1.55	0.54
1:C:307:SER:O	1:D:340:GLU:OE2	2.25	0.54
1:C:458:GLN:HG2	1:C:556:ILE:HG12	1.87	0.54
1:D:362:ASN:OD1	2:D:1002:NAG:N2	2.40	0.54
1:D:401:GLU:O	1:D:405:GLN:N	2.27	0.54
1:D:497:ILE:HG22	1:D:498:HIS:CD2	2.42	0.54
1:D:528:ARG:HH22	1:D:550:HIS:HE1	1.55	0.54
1:B:306:ARG:HD3	1:B:308:PHE:HZ	1.72	0.54
1:B:324:LEU:HD11	1:B:386:TYR:CZ	2.41	0.54
1:C:279:PHE:CZ	1:C:443:VAL:HG21	2.42	0.54
1:D:310:PHE:O	1:D:312:GLU:N	2.40	0.54
1:D:623:VAL:HG22	1:D:624:ASP:O	2.07	0.54
1:A:553:TYR:HA	1:A:556:ILE:HD12	1.90	0.54
1:A:580:ASN:O	1:A:581:ARG:NH1	2.40	0.54
1:D:321:ILE:HG12	1:D:424:ILE:HG12	1.89	0.54
1:D:638:ARG:HE	1:D:643:ASP:CG	2.10	0.54
1:D:639:ILE:HG12	1:D:644:ILE:CG2	2.38	0.54
1:D:688:LYS:O	1:D:692:ALA:N	2.39	0.54
1:A:462:LEU:HD12	1:A:463:ILE:HG23	1.89	0.54
1:A:497:ILE:HG22	1:A:498:HIS:CD2	2.42	0.54
1:A:562:ALA:O	1:A:566:VAL:HG23	2.08	0.54
1:B:280:TRP:HA	1:B:283:THR:HG23	1.90	0.54
1:B:395:LEU:HG	1:B:396:SER:H	1.70	0.54
1:B:553:TYR:HA	1:B:556:ILE:HD12	1.90	0.54
3:C:1006:CHS:OH	3:C:1006:CHS:O	2.23	0.54
1:C:576:PHE:HA	1:C:579:PHE:CE2	2.43	0.54
1:B:456:GLN:OE1	1:C:653:ASN:ND2	2.39	0.54
1:D:224:LEU:O	1:D:228:LEU:N	2.38	0.54
1:A:576:PHE:HA	1:A:579:PHE:CE2	2.43	0.54
1:B:576:PHE:HA	1:B:579:PHE:CE2	2.43	0.54
1:C:435:LEU:HG	1:C:460:LEU:O	2.08	0.54
1:C:497:ILE:HG22	1:C:498:HIS:CD2	2.42	0.54
1:C:639:ILE:HG12	1:C:644:ILE:CG2	2.37	0.54
1:D:553:TYR:HA	1:D:556:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:663:THR:O	1:D:667:PHE:N	2.28	0.54
1:A:226:THR:HB	1:A:483:PHE:HZ	1.71	0.54
1:A:668:MET:HA	1:A:671:ILE:HG22	1.89	0.54
1:B:321:ILE:HG12	1:B:424:ILE:HG12	1.89	0.54
1:C:280:TRP:HA	1:C:283:THR:HG23	1.90	0.54
1:B:497:ILE:HG22	1:B:498:HIS:CD2	2.42	0.54
1:B:668:MET:HA	1:B:671:ILE:HG22	1.89	0.54
1:C:361:ARG:C	2:C:1002:NAG:H81	2.28	0.54
1:C:311:TYR:HB3	1:D:417:ARG:NH1	2.22	0.54
1:C:347:VAL:HG12	1:C:348:TYR:H	1.73	0.54
1:D:279:PHE:CZ	1:D:443:VAL:HG21	2.42	0.54
1:A:306:ARG:HD3	1:A:308:PHE:HZ	1.73	0.54
1:A:347:VAL:HG12	1:A:348:TYR:H	1.73	0.54
1:A:321:ILE:HG12	1:A:424:ILE:HG12	1.89	0.54
1:A:639:ILE:HG12	1:A:644:ILE:CG2	2.38	0.54
1:B:319:PRO:HD2	1:B:395:LEU:HD23	1.89	0.54
1:B:435:LEU:HG	1:B:460:LEU:O	2.07	0.54
1:B:562:ALA:O	1:B:566:VAL:HG23	2.08	0.54
1:B:623:VAL:HG22	1:B:624:ASP:O	2.07	0.54
1:C:321:ILE:HG12	1:C:424:ILE:HG12	1.89	0.54
1:D:435:LEU:HG	1:D:460:LEU:O	2.07	0.54
1:A:280:TRP:HA	1:A:283:THR:HG23	1.90	0.54
1:A:678:ALA:O	1:A:682:ASP:N	2.33	0.54
1:B:347:VAL:HG12	1:B:348:TYR:H	1.73	0.54
1:B:361:ARG:C	2:B:1002:NAG:H81	2.28	0.54
1:B:462:LEU:HD12	1:B:463:ILE:HG23	1.89	0.54
1:D:280:TRP:HA	1:D:283:THR:HG23	1.90	0.54
1:D:309:ILE:HD12	1:D:314:LEU:CA	2.36	0.54
1:A:279:PHE:CZ	1:A:443:VAL:HG21	2.42	0.54
1:B:279:PHE:CZ	1:B:443:VAL:HG21	2.42	0.54
1:D:292:TYR:C	1:D:294:LYS:HZ2	2.11	0.54
1:A:361:ARG:C	2:A:1002:NAG:H81	2.28	0.53
1:A:638:ARG:HE	1:A:643:ASP:CG	2.10	0.53
1:B:252:MET:SD	1:C:448:THR:OG1	2.52	0.53
1:C:553:TYR:HA	1:C:556:ILE:HD12	1.90	0.53
1:D:462:LEU:HD12	1:D:463:ILE:HG23	1.89	0.53
1:A:435:LEU:HG	1:A:460:LEU:O	2.08	0.53
1:B:398:THR:OG1	1:B:400:GLU:OE1	2.16	0.53
1:B:591:SER:HA	1:B:594:ALA:HB3	1.89	0.53
1:B:401:GLU:O	1:B:405:GLN:N	2.27	0.53
1:B:638:ARG:HE	1:B:643:ASP:CG	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:SER:CB	1:C:387:SER:HA	2.39	0.53
1:D:347:VAL:HG12	1:D:348:TYR:H	1.73	0.53
1:C:319:PRO:HD2	1:C:395:LEU:HD23	1.89	0.53
1:C:470:ASP:O	1:C:474:ALA:N	2.22	0.53
1:D:361:ARG:C	2:D:1002:NAG:H81	2.28	0.53
1:D:319:PRO:HD2	1:D:395:LEU:HD23	1.89	0.53
1:A:378:SER:CB	1:A:387:SER:HA	2.39	0.53
1:D:576:PHE:HA	1:D:579:PHE:CE2	2.43	0.53
1:D:668:MET:HA	1:D:671:ILE:HG22	1.89	0.53
1:A:224:LEU:O	1:A:228:LEU:N	2.38	0.53
1:A:539:LEU:CD1	2:A:1004:NAG:O6	2.56	0.53
1:B:539:LEU:CD1	2:B:1004:NAG:O6	2.56	0.53
1:B:293:TRP:CH2	1:B:399:ARG:HG2	2.44	0.53
1:B:688:LYS:O	1:B:692:ALA:N	2.39	0.53
1:D:562:ALA:O	1:D:566:VAL:HG23	2.08	0.53
1:A:319:PRO:HD2	1:A:395:LEU:HD23	1.89	0.53
1:B:616:TYR:O	1:B:620:GLY:N	2.42	0.53
1:D:674:ASN:OD1	1:D:678:ALA:N	2.42	0.53
1:C:539:LEU:CD1	2:C:1004:NAG:O6	2.56	0.53
1:C:623:VAL:HG22	1:C:624:ASP:O	2.07	0.53
1:D:378:SER:CB	1:D:387:SER:HA	2.39	0.53
5:A:1010:PLM:O2	3:D:1005:CHS:N	2.42	0.53
1:C:428:VAL:O	1:C:437:CYS:N	2.36	0.53
1:C:462:LEU:HD12	1:C:463:ILE:HG23	1.89	0.53
1:A:428:VAL:O	1:A:437:CYS:N	2.36	0.53
1:A:674:ASN:OD1	1:A:678:ALA:N	2.42	0.53
1:C:562:ALA:O	1:C:566:VAL:HG23	2.08	0.53
1:C:674:ASN:OD1	1:C:678:ALA:N	2.42	0.53
1:D:519:VAL:HA	1:D:522:ILE:HB	1.91	0.53
1:D:624:ASP:C	1:D:626:PHE:H	2.12	0.53
1:A:293:TRP:CH2	1:A:399:ARG:HG2	2.44	0.52
1:B:378:SER:CB	1:B:387:SER:HA	2.39	0.52
1:B:445:PHE:CE1	1:B:451:VAL:HG22	2.44	0.52
1:B:466:VAL:N	1:B:470:ASP:HB2	2.16	0.52
1:B:639:ILE:HG12	1:B:644:ILE:CG2	2.37	0.52
1:C:519:VAL:HA	1:C:522:ILE:HB	1.91	0.52
1:D:616:TYR:O	1:D:620:GLY:N	2.42	0.52
1:C:293:TRP:CH2	1:C:399:ARG:HG2	2.44	0.52
1:C:445:PHE:CE1	1:C:451:VAL:HG22	2.44	0.52
1:D:294:LYS:HE2	1:D:309:ILE:CA	2.38	0.52
1:D:678:ALA:O	1:D:682:ASP:N	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:THR:OG1	1:D:335:GLN:OE1	2.27	0.52
1:D:539:LEU:CD1	2:D:1004:NAG:O6	2.56	0.52
1:A:519:VAL:HA	1:A:522:ILE:HB	1.91	0.52
1:B:249:TYR:HE1	1:B:313:ASN:HD21	1.58	0.52
4:C:1007:PX6:H41	1:D:655:VAL:HG11	1.92	0.52
1:C:616:TYR:O	1:C:620:GLY:N	2.42	0.52
1:D:445:PHE:CE1	1:D:451:VAL:HG22	2.44	0.52
1:A:362:ASN:CG	2:A:1002:NAG:C7	2.78	0.52
1:B:678:ALA:O	1:B:682:ASP:N	2.32	0.52
1:C:624:ASP:C	1:C:626:PHE:H	2.12	0.52
1:D:657:GLY:O	1:D:659:ILE:N	2.43	0.52
1:A:361:ARG:HD3	1:A:366:TRP:CD1	2.45	0.52
1:B:362:ASN:CG	2:B:1002:NAG:C7	2.78	0.52
1:B:692:ALA:HA	1:B:695:LYS:HG2	1.92	0.52
1:C:362:ASN:CG	2:C:1002:NAG:C7	2.78	0.52
1:D:528:ARG:HH12	1:D:550:HIS:CE1	2.28	0.52
1:A:528:ARG:HH12	1:A:550:HIS:CE1	2.28	0.52
1:A:659:ILE:O	1:A:663:THR:HG23	2.10	0.52
1:B:306:ARG:CG	1:B:308:PHE:CZ	2.89	0.52
1:C:261:PRO:HA	1:C:269:ASN:HA	1.92	0.52
1:C:663:THR:O	1:C:667:PHE:N	2.28	0.52
1:A:398:THR:O	1:A:398:THR:CG2	2.58	0.52
1:A:657:GLY:O	1:A:659:ILE:N	2.43	0.52
1:B:361:ARG:HD3	1:B:366:TRP:CD1	2.45	0.52
1:B:519:VAL:HA	1:B:522:ILE:HB	1.91	0.52
1:B:624:ASP:C	1:B:626:PHE:H	2.12	0.52
1:D:261:PRO:HA	1:D:269:ASN:HA	1.92	0.52
1:D:359:GLY:HA2	1:D:366:TRP:CD1	2.45	0.52
1:D:398:THR:O	1:D:398:THR:CG2	2.58	0.52
1:D:580:ASN:O	1:D:581:ARG:NH1	2.40	0.52
1:A:683:THR:O	1:A:687:VAL:N	2.43	0.52
1:B:683:THR:O	1:B:687:VAL:N	2.43	0.52
1:D:362:ASN:CG	2:D:1002:NAG:C7	2.78	0.52
1:D:692:ALA:HA	1:D:695:LYS:HG2	1.92	0.52
1:A:445:PHE:CE1	1:A:451:VAL:HG22	2.44	0.52
1:B:674:ASN:OD1	1:B:678:ALA:N	2.42	0.52
1:C:659:ILE:O	1:C:663:THR:HG23	2.10	0.52
1:B:379:HIS:HB3	1:B:423:PHE:CZ	2.45	0.51
1:C:361:ARG:HD3	1:C:366:TRP:CD1	2.45	0.51
1:D:275:SER:HB2	1:D:278:ASP:CG	2.31	0.51
1:D:327:ARG:HD3	1:D:354:ASP:OD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:ARG:HD3	1:D:366:TRP:CD1	2.45	0.51
1:D:683:THR:O	1:D:687:VAL:N	2.43	0.51
1:A:249:TYR:HE1	1:A:313:ASN:HD21	1.58	0.51
1:A:616:TYR:O	1:A:620:GLY:N	2.42	0.51
1:A:624:ASP:C	1:A:626:PHE:H	2.12	0.51
1:B:261:PRO:HA	1:B:269:ASN:HA	1.92	0.51
1:B:657:GLY:O	1:B:659:ILE:N	2.43	0.51
1:C:379:HIS:HB3	1:C:423:PHE:CZ	2.45	0.51
1:C:364:THR:HG23	1:C:392:TYR:CZ	2.46	0.51
1:C:516:VAL:O	1:C:520:VAL:HG23	2.11	0.51
1:C:528:ARG:HH12	1:C:550:HIS:CE1	2.28	0.51
1:D:293:TRP:CH2	1:D:399:ARG:HG2	2.44	0.51
1:B:327:ARG:HD3	1:B:354:ASP:OD2	2.10	0.51
1:B:364:THR:HG23	1:B:392:TYR:CZ	2.46	0.51
1:B:428:VAL:O	1:B:437:CYS:N	2.36	0.51
1:B:634:PHE:O	1:B:637:PHE:N	2.44	0.51
1:C:275:SER:HB2	1:C:278:ASP:CG	2.31	0.51
1:C:657:GLY:O	1:C:659:ILE:N	2.43	0.51
1:D:309:ILE:HD12	1:D:314:LEU:N	2.08	0.51
1:A:275:SER:HB2	1:A:278:ASP:CG	2.31	0.51
1:A:573:LEU:O	1:A:577:ILE:N	2.33	0.51
1:B:311:TYR:HB3	1:C:417:ARG:NH1	2.24	0.51
1:B:659:ILE:O	1:B:663:THR:HG23	2.10	0.51
1:B:684:TYR:HA	1:B:687:VAL:HG13	1.93	0.51
1:C:359:GLY:HA2	1:C:366:TRP:CD1	2.45	0.51
1:C:480:PHE:O	1:C:484:ILE:HD12	2.11	0.51
1:A:400:GLU:N	1:A:400:GLU:OE1	2.36	0.51
1:B:275:SER:HB2	1:B:278:ASP:CG	2.30	0.51
1:B:398:THR:O	1:B:398:THR:CG2	2.58	0.51
1:B:528:ARG:HH12	1:B:550:HIS:CE1	2.28	0.51
1:B:570:TRP:O	1:B:573:LEU:HG	2.11	0.51
1:C:249:TYR:HE1	1:C:313:ASN:HD21	1.58	0.51
1:C:570:TRP:O	1:C:573:LEU:HG	2.11	0.51
3:D:1006:CHS:OH	3:D:1006:CHS:O	2.24	0.51
1:D:364:THR:HG23	1:D:392:TYR:CZ	2.46	0.51
1:D:430:ASN:OD1	1:D:435:LEU:N	2.43	0.51
1:D:516:VAL:O	1:D:520:VAL:HG23	2.11	0.51
1:A:364:THR:HG23	1:A:392:TYR:CZ	2.46	0.51
1:A:430:ASN:OD1	1:A:435:LEU:N	2.43	0.51
1:A:541:ASP:OD1	1:A:542:GLN:N	2.44	0.51
1:B:430:ASN:OD1	1:B:435:LEU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LEU:O	1:C:228:LEU:N	2.38	0.51
1:C:279:PHE:O	1:C:282:PHE:HB3	2.11	0.51
1:C:430:ASN:OD1	1:C:435:LEU:N	2.43	0.51
1:C:683:THR:O	1:C:687:VAL:N	2.43	0.51
1:D:294:LYS:HD3	1:D:308:PHE:O	2.10	0.51
1:A:261:PRO:HA	1:A:269:ASN:HA	1.92	0.51
1:A:359:GLY:HA2	1:A:366:TRP:CD1	2.45	0.51
1:A:639:ILE:HG12	1:A:644:ILE:HG21	1.93	0.51
1:C:514:ILE:HA	1:C:517:LEU:HD12	1.92	0.51
1:A:606:ILE:HD13	1:D:573:LEU:HD11	1.60	0.51
1:A:675:MET:O	1:A:679:ILE:HD12	2.11	0.51
3:A:1005:CHS:N	5:B:1010:PLM:O2	2.44	0.51
1:B:514:ILE:HA	1:B:517:LEU:HD12	1.93	0.51
1:D:555:GLN:HA	1:D:558:PHE:HB3	1.93	0.51
1:A:516:VAL:O	1:A:520:VAL:HG23	2.11	0.51
1:A:573:LEU:HA	1:A:576:PHE:HB2	1.93	0.51
1:A:616:TYR:OH	1:D:244:SER:HA	2.10	0.51
1:B:294:LYS:HD3	1:B:308:PHE:O	2.11	0.51
1:B:359:GLY:HA2	1:B:366:TRP:CD1	2.45	0.51
1:C:634:PHE:O	1:C:637:PHE:N	2.43	0.51
1:D:279:PHE:O	1:D:282:PHE:HB3	2.11	0.51
1:D:541:ASP:OD1	1:D:542:GLN:N	2.44	0.51
1:D:659:ILE:O	1:D:663:THR:HG23	2.10	0.51
1:A:279:PHE:O	1:A:282:PHE:HB3	2.11	0.51
1:A:692:ALA:HA	1:A:695:LYS:HG2	1.92	0.51
1:A:247:TYR:HE1	1:B:623:VAL:C	2.14	0.51
1:A:379:HIS:HB3	1:A:423:PHE:CZ	2.45	0.50
1:A:463:ILE:HG13	1:A:465:TYR:O	2.11	0.50
1:A:570:TRP:O	1:A:573:LEU:HG	2.11	0.50
1:A:611:TYR:HB3	1:A:660:TYR:HE1	1.76	0.50
1:B:279:PHE:O	1:B:282:PHE:HB3	2.11	0.50
1:B:331:CYS:HB3	1:B:346:ASP:HB3	1.94	0.50
1:B:555:GLN:HA	1:B:558:PHE:HB3	1.93	0.50
1:C:639:ILE:HG12	1:C:644:ILE:HG21	1.92	0.50
1:D:254:SER:O	1:D:257:PHE:N	2.40	0.50
1:D:463:ILE:HG13	1:D:465:TYR:O	2.11	0.50
1:D:634:PHE:O	1:D:637:PHE:N	2.43	0.50
1:D:684:TYR:HA	1:D:687:VAL:HG13	1.93	0.50
1:A:331:CYS:HB3	1:A:346:ASP:HB3	1.94	0.50
1:A:327:ARG:HD3	1:A:354:ASP:OD2	2.10	0.50
1:B:573:LEU:HA	1:B:576:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:LEU:O	1:C:577:ILE:N	2.33	0.50
1:C:684:TYR:HA	1:C:687:VAL:HG13	1.93	0.50
1:C:692:ALA:HA	1:C:695:LYS:HG2	1.92	0.50
1:D:288:LEU:HD11	1:D:402:THR:HG23	1.93	0.50
1:A:480:PHE:O	1:A:484:ILE:HD12	2.11	0.50
1:B:436:PHE:HB3	1:B:460:LEU:HB3	1.93	0.50
1:B:480:PHE:O	1:B:484:ILE:HD12	2.11	0.50
1:B:611:TYR:HB3	1:B:660:TYR:HE1	1.76	0.50
1:D:249:TYR:HE1	1:D:313:ASN:HD21	1.58	0.50
1:D:379:HIS:HB3	1:D:423:PHE:CZ	2.45	0.50
1:D:480:PHE:O	1:D:484:ILE:HD12	2.11	0.50
1:D:570:TRP:O	1:D:573:LEU:HG	2.11	0.50
1:D:573:LEU:O	1:D:577:ILE:N	2.33	0.50
1:B:322:ARG:N	1:B:423:PHE:O	2.28	0.50
1:B:532:VAL:HG21	1:B:551:LEU:HD21	1.94	0.50
1:B:541:ASP:OD1	1:B:542:GLN:N	2.44	0.50
1:B:573:LEU:O	1:B:577:ILE:N	2.33	0.50
1:C:327:ARG:HD3	1:C:354:ASP:OD2	2.10	0.50
1:B:432:ASN:ND2	1:C:447:ALA:O	2.41	0.50
1:C:463:ILE:HG13	1:C:465:TYR:O	2.11	0.50
1:C:532:VAL:HG21	1:C:551:LEU:HD21	1.94	0.50
1:B:516:VAL:O	1:B:520:VAL:HG23	2.11	0.50
1:C:398:THR:O	1:C:398:THR:CG2	2.58	0.50
1:A:448:THR:HB	1:D:249:TYR:HD1	1.76	0.50
1:D:436:PHE:HB3	1:D:460:LEU:HB3	1.93	0.50
1:D:611:TYR:HB3	1:D:660:TYR:HE1	1.76	0.50
1:A:634:PHE:O	1:A:637:PHE:N	2.44	0.50
1:B:580:ASN:O	1:B:581:ARG:NH1	2.40	0.50
1:C:361:ARG:C	2:C:1002:NAG:C8	2.79	0.50
1:B:224:LEU:O	1:B:228:LEU:N	2.38	0.50
1:B:675:MET:O	1:B:679:ILE:HD12	2.11	0.50
1:C:541:ASP:OD1	1:C:542:GLN:N	2.44	0.50
1:D:314:LEU:HB3	1:D:429:TYR:CD2	2.26	0.50
1:D:331:CYS:HB3	1:D:346:ASP:HB3	1.94	0.50
1:C:244:SER:HA	1:D:616:TYR:OH	2.11	0.50
1:D:639:ILE:HG12	1:D:644:ILE:HG21	1.93	0.50
1:B:639:ILE:HG12	1:B:644:ILE:HG21	1.92	0.50
1:C:555:GLN:HA	1:C:558:PHE:HB3	1.93	0.50
1:D:532:VAL:HG21	1:D:551:LEU:HD21	1.94	0.50
1:D:675:MET:O	1:D:679:ILE:HD12	2.11	0.50
1:A:684:TYR:HA	1:A:687:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LEU:HD11	1:B:402:THR:HG23	1.93	0.50
1:C:331:CYS:HB3	1:C:346:ASP:HB3	1.93	0.50
1:C:401:GLU:HA	1:C:404:ALA:HB3	1.93	0.50
1:C:611:TYR:HB3	1:C:660:TYR:HE1	1.76	0.50
1:A:532:VAL:HG21	1:A:551:LEU:HD21	1.94	0.49
1:C:677:LEU:O	1:D:674:ASN:ND2	2.45	0.49
1:C:675:MET:O	1:C:679:ILE:HD12	2.11	0.49
1:D:294:LYS:NZ	1:D:308:PHE:O	2.41	0.49
1:A:288:LEU:HD11	1:A:402:THR:HG23	1.93	0.49
1:A:555:GLN:HA	1:A:558:PHE:HB3	1.93	0.49
1:A:577:ILE:HG12	1:B:602:ILE:HD13	1.94	0.49
1:C:307:SER:N	1:D:340:GLU:OE2	2.44	0.49
1:D:466:VAL:H	1:D:470:ASP:CB	2.20	0.49
1:D:603:MET:O	1:D:606:ILE:HG22	2.12	0.49
1:A:254:SER:O	1:A:257:PHE:N	2.39	0.49
1:A:514:ILE:HA	1:A:517:LEU:HD12	1.93	0.49
1:C:580:ASN:O	1:C:581:ARG:NH1	2.40	0.49
1:D:309:ILE:HD12	1:D:314:LEU:HA	1.94	0.49
3:C:1005:CHS:N	5:D:1010:PLM:O2	2.45	0.49
1:C:331:CYS:SG	1:C:332:SER:N	2.83	0.49
1:C:567:PHE:O	1:C:571:ILE:HG23	2.13	0.49
1:A:447:ALA:O	1:D:432:ASN:ND2	2.44	0.49
1:A:436:PHE:HB3	1:A:460:LEU:HB3	1.93	0.49
1:A:683:THR:O	1:A:687:VAL:HG13	2.13	0.49
1:B:401:GLU:HA	1:B:404:ALA:HB3	1.94	0.49
1:B:677:LEU:HD22	1:C:674:ASN:HB2	1.94	0.49
1:C:409:LEU:O	1:C:413:VAL:N	2.46	0.49
1:D:567:PHE:O	1:D:571:ILE:HG23	2.13	0.49
1:D:573:LEU:HA	1:D:576:PHE:HB2	1.93	0.49
1:A:309:ILE:HG12	1:A:314:LEU:HA	1.94	0.49
1:B:280:TRP:NE1	1:B:414:TRP:CD1	2.81	0.49
1:B:463:ILE:HG13	1:B:465:TYR:O	2.11	0.49
1:D:409:LEU:O	1:D:413:VAL:N	2.46	0.49
1:A:601:ALA:HB1	1:A:605:PHE:CZ	2.48	0.49
1:A:663:THR:O	1:A:667:PHE:N	2.28	0.49
1:C:280:TRP:NE1	1:C:414:TRP:CD1	2.81	0.49
1:C:573:LEU:HA	1:C:576:PHE:HB2	1.93	0.49
1:D:252:MET:HG3	1:D:253:MET:N	2.28	0.49
1:A:401:GLU:HA	1:A:404:ALA:HB3	1.93	0.49
3:B:1005:CHS:N	5:C:1010:PLM:O2	2.45	0.49
1:B:331:CYS:SG	1:B:332:SER:N	2.83	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:PHE:CZ	1:B:484:ILE:HD11	2.48	0.49
1:B:683:THR:O	1:B:687:VAL:HG13	2.13	0.49
1:C:399:ARG:HD3	1:C:402:THR:HG21	1.95	0.49
1:C:436:PHE:HB3	1:C:460:LEU:HB3	1.93	0.49
1:C:603:MET:O	1:C:606:ILE:HG22	2.13	0.49
1:D:401:GLU:HA	1:D:404:ALA:HB3	1.94	0.49
1:D:514:ILE:HA	1:D:517:LEU:HD12	1.93	0.49
1:A:335:GLN:OE1	1:D:467:THR:OG1	2.30	0.49
1:B:409:LEU:O	1:B:413:VAL:N	2.46	0.49
1:C:249:TYR:HD1	1:D:448:THR:HB	1.76	0.49
1:A:230:PHE:CZ	1:A:484:ILE:HD11	2.48	0.49
1:A:409:LEU:O	1:A:413:VAL:N	2.46	0.49
1:B:573:LEU:O	1:B:577:ILE:HG22	2.13	0.49
4:C:1007:PX6:H24	5:C:1010:PLM:HG2	1.95	0.49
1:C:307:SER:HB3	1:C:397:ARG:HH21	1.77	0.49
1:C:322:ARG:N	1:C:423:PHE:O	2.28	0.49
1:C:683:THR:O	1:C:687:VAL:HG13	2.13	0.49
1:D:230:PHE:CZ	1:D:484:ILE:HD11	2.48	0.49
1:D:513:VAL:O	1:D:517:LEU:HG	2.13	0.49
1:A:602:ILE:HD13	1:D:577:ILE:HG12	1.95	0.49
1:A:252:MET:HG3	1:A:253:MET:N	2.28	0.48
1:A:567:PHE:O	1:A:571:ILE:HG23	2.13	0.48
1:B:309:ILE:HG12	1:B:314:LEU:HA	1.94	0.48
1:C:601:ALA:HB1	1:C:605:PHE:CZ	2.48	0.48
1:D:399:ARG:HD3	1:D:402:THR:HG21	1.95	0.48
1:D:601:ALA:HB1	1:D:605:PHE:CZ	2.48	0.48
1:A:513:VAL:HG12	1:A:517:LEU:HD11	1.95	0.48
1:B:361:ARG:C	2:B:1002:NAG:C8	2.80	0.48
1:B:567:PHE:O	1:B:571:ILE:HG23	2.13	0.48
1:C:573:LEU:O	1:C:577:ILE:HG22	2.13	0.48
1:D:683:THR:O	1:D:687:VAL:HG13	2.13	0.48
1:B:532:VAL:O	1:B:536:LEU:HD13	2.14	0.48
1:B:601:ALA:HB1	1:B:605:PHE:CZ	2.48	0.48
1:C:252:MET:HG3	1:C:253:MET:N	2.28	0.48
1:C:288:LEU:HD11	1:C:402:THR:HG23	1.93	0.48
1:D:280:TRP:NE1	1:D:414:TRP:CD1	2.81	0.48
1:D:428:VAL:O	1:D:437:CYS:N	2.36	0.48
1:A:322:ARG:N	1:A:423:PHE:O	2.28	0.48
1:A:513:VAL:O	1:A:517:LEU:HG	2.13	0.48
1:B:513:VAL:O	1:B:517:LEU:HG	2.13	0.48
1:B:603:MET:O	1:B:606:ILE:HG22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:PHE:CZ	1:C:484:ILE:HD11	2.48	0.48
1:C:238:THR:HA	1:C:241:MET:HG2	1.95	0.48
1:D:269:ASN:ND2	1:D:271:LYS:HB3	2.29	0.48
1:D:573:LEU:O	1:D:577:ILE:HG22	2.13	0.48
4:A:1007:PX6:H53	4:A:1007:PX6:H46	1.60	0.48
1:A:399:ARG:HD3	1:A:402:THR:HG21	1.95	0.48
1:A:406:VAL:HG13	1:A:414:TRP:NE1	2.24	0.48
1:A:624:ASP:C	1:A:626:PHE:N	2.67	0.48
1:B:269:ASN:ND2	1:B:271:LYS:HB3	2.29	0.48
1:B:640:ILE:HD12	1:B:672:LEU:CD2	2.44	0.48
1:C:249:TYR:CD1	1:D:448:THR:HB	2.48	0.48
1:C:269:ASN:ND2	1:C:271:LYS:HB3	2.29	0.48
1:C:319:PRO:HA	1:C:426:PHE:HB3	1.95	0.48
1:C:430:ASN:ND2	1:C:435:LEU:HB3	2.27	0.48
1:C:513:VAL:HG12	1:C:517:LEU:HD11	1.95	0.48
1:D:238:THR:HA	1:D:241:MET:HG2	1.96	0.48
1:D:640:ILE:HD12	1:D:672:LEU:CD2	2.44	0.48
1:A:223:GLU:OE1	1:A:227:TYR:CE2	2.66	0.48
1:A:238:THR:HA	1:A:241:MET:HG2	1.95	0.48
1:B:238:THR:HA	1:B:241:MET:HG2	1.96	0.48
1:B:513:VAL:HG12	1:B:517:LEU:HD11	1.95	0.48
5:C:1009:PLM:H61	5:C:1009:PLM:H92	1.73	0.48
1:D:223:GLU:OE1	1:D:227:TYR:CE2	2.66	0.48
1:A:332:SER:HB3	1:D:432:ASN:HA	1.95	0.48
1:D:513:VAL:HG12	1:D:517:LEU:HD11	1.95	0.48
1:A:323:GLN:NE2	1:A:415:LEU:O	2.44	0.48
1:B:223:GLU:OE1	1:B:227:TYR:CE2	2.66	0.48
1:C:223:GLU:OE1	1:C:227:TYR:CE2	2.66	0.48
1:C:577:ILE:HG12	1:D:602:ILE:HD13	1.96	0.48
1:D:294:LYS:HZ1	1:D:309:ILE:HA	1.71	0.48
1:A:603:MET:O	1:A:606:ILE:HG22	2.13	0.48
1:B:689:SER:HA	1:B:692:ALA:HB3	1.96	0.48
1:C:532:VAL:O	1:C:536:LEU:HD13	2.14	0.48
1:A:308:PHE:CD1	1:A:308:PHE:N	2.80	0.48
1:A:487:TYR:HD1	1:A:490:GLU:OE2	1.97	0.48
1:A:615:ALA:HA	1:A:619:PHE:CD2	2.49	0.48
1:A:640:ILE:HD12	1:A:672:LEU:CD2	2.44	0.48
1:B:466:VAL:H	1:B:470:ASP:CB	2.20	0.48
1:B:487:TYR:HD1	1:B:490:GLU:OE2	1.97	0.48
1:C:279:PHE:CE1	1:C:443:VAL:HG11	2.49	0.48
1:D:275:SER:HB2	1:D:278:ASP:OD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:639:ILE:O	1:D:642:GLY:N	2.47	0.48
1:A:280:TRP:NE1	1:A:414:TRP:CD1	2.81	0.48
1:A:279:PHE:CE1	1:A:443:VAL:HG11	2.49	0.48
1:A:573:LEU:O	1:A:577:ILE:HG22	2.13	0.48
1:B:249:TYR:HD1	1:C:448:THR:HB	1.79	0.48
1:B:323:GLN:NE2	1:B:415:LEU:O	2.44	0.48
1:C:689:SER:HA	1:C:692:ALA:HB3	1.95	0.48
1:D:331:CYS:SG	1:D:332:SER:N	2.83	0.48
1:D:279:PHE:CE1	1:D:443:VAL:HG11	2.48	0.48
1:B:254:SER:O	1:B:257:PHE:N	2.39	0.47
1:B:279:PHE:CE1	1:B:443:VAL:HG11	2.49	0.47
1:B:639:ILE:O	1:B:642:GLY:N	2.47	0.47
1:C:323:GLN:NE2	1:C:415:LEU:O	2.44	0.47
1:C:487:TYR:HD1	1:C:490:GLU:OE2	1.97	0.47
1:D:398:THR:CB	2:D:1001:NAG:C6	2.85	0.47
1:D:319:PRO:HA	1:D:426:PHE:HB3	1.96	0.47
1:D:487:TYR:HD1	1:D:490:GLU:OE2	1.97	0.47
1:A:571:ILE:O	1:A:574:PHE:HB3	2.14	0.47
1:A:604:PHE:O	1:A:607:ILE:HG22	2.14	0.47
1:A:639:ILE:O	1:A:642:GLY:N	2.47	0.47
1:B:399:ARG:HD3	1:B:402:THR:HG21	1.95	0.47
1:B:309:ILE:O	1:B:312:GLU:N	2.42	0.47
1:B:406:VAL:HG13	1:B:414:TRP:NE1	2.24	0.47
1:B:571:ILE:O	1:B:574:PHE:HB3	2.14	0.47
1:C:275:SER:HB2	1:C:278:ASP:OD2	2.14	0.47
1:C:513:VAL:O	1:C:517:LEU:HG	2.13	0.47
1:C:571:ILE:O	1:C:574:PHE:HB3	2.14	0.47
1:C:624:ASP:C	1:C:626:PHE:N	2.67	0.47
1:C:639:ILE:O	1:C:642:GLY:N	2.47	0.47
1:D:689:SER:HA	1:D:692:ALA:HB3	1.95	0.47
1:A:275:SER:HB2	1:A:278:ASP:OD2	2.14	0.47
1:A:466:VAL:H	1:A:470:ASP:CB	2.20	0.47
1:B:252:MET:HG3	1:B:253:MET:N	2.28	0.47
1:B:379:HIS:HA	1:B:440:ARG:NH2	2.29	0.47
1:B:400:GLU:OE1	1:B:400:GLU:N	2.36	0.47
1:C:573:LEU:HD12	1:D:606:ILE:HD13	1.89	0.47
1:B:624:ASP:C	1:B:626:PHE:N	2.67	0.47
1:D:619:PHE:C	1:D:621:THR:N	2.67	0.47
1:A:532:VAL:O	1:A:536:LEU:HD13	2.14	0.47
1:A:582:THR:O	1:A:586:LEU:HG	2.15	0.47
1:B:604:PHE:O	1:B:607:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:HIS:HA	1:C:440:ARG:NH2	2.29	0.47
1:C:524:ILE:HA	1:C:527:TYR:HB3	1.97	0.47
1:C:582:THR:O	1:C:586:LEU:HG	2.15	0.47
1:D:604:PHE:O	1:D:607:ILE:HG22	2.14	0.47
1:A:674:ASN:ND2	1:D:677:LEU:O	2.47	0.47
1:A:319:PRO:HA	1:A:426:PHE:HB3	1.96	0.47
1:A:248:TYR:CE2	1:B:452:ILE:HD12	2.50	0.47
1:B:615:ALA:HA	1:B:619:PHE:CD2	2.49	0.47
1:C:401:GLU:O	1:C:405:GLN:N	2.27	0.47
1:C:641:LEU:HD21	1:D:642:GLY:HA2	1.96	0.47
1:D:379:HIS:HA	1:D:440:ARG:NH2	2.29	0.47
1:D:571:ILE:O	1:D:574:PHE:HB3	2.14	0.47
1:D:582:THR:O	1:D:586:LEU:HG	2.15	0.47
1:D:656:LEU:HA	1:D:657:GLY:HA2	1.34	0.47
1:A:269:ASN:ND2	1:A:271:LYS:HB3	2.29	0.47
1:A:323:GLN:HE22	1:A:415:LEU:HB2	1.79	0.47
1:A:627:SER:HB3	1:D:247:TYR:HB2	1.97	0.47
1:B:582:THR:O	1:B:586:LEU:HG	2.15	0.47
1:B:630:GLN:O	1:B:633:ILE:HG22	2.15	0.47
4:C:1007:PX6:H46	4:C:1007:PX6:H53	1.63	0.47
1:C:612:ALA:HB2	1:C:636:GLN:OE1	2.15	0.47
1:C:640:ILE:HD12	1:C:672:LEU:CD2	2.44	0.47
1:B:677:LEU:O	1:C:674:ASN:ND2	2.45	0.47
4:D:1007:PX6:H24	5:D:1010:PLM:HG2	1.96	0.47
1:A:417:ARG:HH11	1:D:311:TYR:HB3	1.78	0.47
1:D:382:ILE:HG23	1:D:383:ILE:N	2.30	0.47
1:D:323:GLN:HE22	1:D:415:LEU:HB2	1.80	0.47
1:D:430:ASN:ND2	1:D:435:LEU:HB3	2.27	0.47
1:D:501:HIS:O	1:D:505:SER:OG	2.33	0.47
1:A:252:MET:SD	1:B:448:THR:OG1	2.60	0.47
1:B:663:THR:O	1:B:667:PHE:N	2.28	0.47
1:C:605:PHE:HZ	5:C:1009:PLM:HG3	1.80	0.47
1:C:652:ALA:O	1:C:653:ASN:ND2	2.48	0.47
1:A:448:THR:HB	1:D:249:TYR:CD1	2.50	0.47
1:A:652:ALA:O	1:A:653:ASN:ND2	2.48	0.47
1:C:501:HIS:O	1:C:505:SER:OG	2.33	0.47
1:C:630:GLN:O	1:C:633:ILE:HG22	2.15	0.47
1:D:624:ASP:C	1:D:626:PHE:N	2.67	0.47
1:D:630:GLN:O	1:D:633:ILE:HG22	2.15	0.47
1:A:524:ILE:HA	1:A:527:TYR:HB3	1.97	0.47
1:A:689:SER:HA	1:A:692:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:SER:HB2	1:B:278:ASP:OD2	2.14	0.47
1:B:430:ASN:ND2	1:B:435:LEU:HB3	2.27	0.47
1:A:244:SER:HA	1:B:616:TYR:OH	2.14	0.47
1:B:652:ALA:O	1:B:653:ASN:ND2	2.48	0.47
1:D:532:VAL:O	1:D:536:LEU:HD13	2.14	0.47
1:A:465:TYR:HA	1:A:470:ASP:OD2	2.15	0.46
3:B:1005:CHS:HD22	3:B:1006:CHS:HD23	1.98	0.46
1:B:382:ILE:HG23	1:B:383:ILE:N	2.30	0.46
1:D:652:ALA:O	1:D:653:ASN:ND2	2.48	0.46
1:A:379:HIS:HA	1:A:440:ARG:NH2	2.29	0.46
4:B:1007:PX6:H24	5:B:1010:PLM:HG2	1.97	0.46
1:D:406:VAL:HG13	1:D:414:TRP:NE1	2.24	0.46
1:A:382:ILE:HG23	1:A:383:ILE:N	2.30	0.46
1:B:612:ALA:HB2	1:B:636:GLN:OE1	2.15	0.46
1:D:406:VAL:O	1:D:410:LYS:N	2.47	0.46
1:A:325:ARG:NH2	1:A:355:ARG:HA	2.29	0.46
1:A:548:PHE:O	1:A:551:LEU:HB2	2.16	0.46
1:A:630:GLN:O	1:A:633:ILE:HG22	2.15	0.46
1:A:612:ALA:HB2	1:A:636:GLN:OE1	2.15	0.46
1:B:524:ILE:HA	1:B:527:TYR:HB3	1.97	0.46
1:C:323:GLN:HE22	1:C:415:LEU:HB2	1.80	0.46
1:D:615:ALA:HA	1:D:619:PHE:CD2	2.49	0.46
1:C:247:TYR:HB2	1:D:627:SER:HB3	1.98	0.46
1:A:328:ASN:OD1	1:A:343:GLU:HB3	2.15	0.46
1:B:249:TYR:CD1	1:C:448:THR:HB	2.51	0.46
1:C:604:PHE:O	1:C:607:ILE:HG22	2.14	0.46
1:B:244:SER:HA	1:C:616:TYR:OH	2.16	0.46
1:B:323:GLN:HE22	1:B:415:LEU:HB2	1.80	0.46
1:C:248:TYR:C	1:C:252:MET:HG2	2.36	0.46
1:C:465:TYR:HA	1:C:470:ASP:OD2	2.16	0.46
1:C:548:PHE:O	1:C:551:LEU:HB2	2.16	0.46
1:C:247:TYR:HB2	1:D:627:SER:CB	2.45	0.46
1:A:331:CYS:SG	1:A:332:SER:N	2.83	0.46
1:A:605:PHE:HZ	5:A:1009:PLM:HG3	1.79	0.46
1:B:294:LYS:HD2	1:B:294:LYS:N	2.31	0.46
1:B:325:ARG:NH2	1:B:355:ARG:HA	2.29	0.46
1:B:319:PRO:HA	1:B:426:PHE:HB3	1.96	0.46
1:C:294:LYS:HD2	1:C:294:LYS:N	2.31	0.46
1:C:332:SER:HB2	1:C:344:CYS:HB3	1.98	0.46
1:C:619:PHE:C	1:C:621:THR:N	2.67	0.46
1:D:332:SER:HB2	1:D:344:CYS:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:ALA:CA	1:D:385:THR:HG22	2.35	0.46
1:D:441:LEU:HA	1:D:441:LEU:HD23	1.74	0.46
1:B:577:ILE:HG12	1:C:602:ILE:CD1	2.45	0.46
1:C:615:ALA:HA	1:C:619:PHE:CD2	2.49	0.46
5:D:1009:PLM:H71	5:D:1009:PLM:H42	1.60	0.46
1:D:465:TYR:HA	1:D:470:ASP:OD2	2.15	0.46
1:A:309:ILE:HD11	1:A:314:LEU:C	2.28	0.46
1:A:332:SER:HB2	1:A:344:CYS:HB3	1.98	0.46
1:B:223:GLU:OE1	1:B:227:TYR:HE2	1.99	0.46
1:B:248:TYR:C	1:B:252:MET:HG2	2.36	0.46
1:B:465:TYR:HA	1:B:470:ASP:OD2	2.15	0.46
1:D:223:GLU:OE1	1:D:227:TYR:HE2	1.99	0.46
1:D:328:ASN:ND2	1:D:343:GLU:OE1	2.49	0.46
1:D:524:ILE:HA	1:D:527:TYR:HB3	1.97	0.46
1:A:223:GLU:OE1	1:A:227:TYR:HE2	1.99	0.46
5:B:1010:PLM:H71	5:B:1010:PLM:H42	1.56	0.46
1:B:573:LEU:HD12	1:C:606:ILE:HD13	1.83	0.46
1:C:293:TRP:CZ3	1:C:399:ARG:HG2	2.51	0.46
1:D:294:LYS:HE2	1:D:309:ILE:HA	1.98	0.46
1:D:293:TRP:CZ3	1:D:399:ARG:HG2	2.51	0.46
1:A:619:PHE:C	1:A:621:THR:N	2.67	0.45
1:C:223:GLU:OE1	1:C:227:TYR:HE2	1.99	0.45
1:C:382:ILE:HG23	1:C:383:ILE:N	2.30	0.45
1:C:466:VAL:H	1:C:470:ASP:CB	2.20	0.45
1:C:561:ILE:O	1:C:565:THR:HG23	2.17	0.45
1:D:328:ASN:OD1	1:D:343:GLU:HB3	2.15	0.45
1:A:294:LYS:N	1:A:294:LYS:HD2	2.31	0.45
1:A:328:ASN:ND2	1:A:343:GLU:OE1	2.49	0.45
1:B:247:TYR:HE1	1:C:623:VAL:C	2.19	0.45
1:B:458:GLN:HE21	1:B:459:PRO:HD2	1.81	0.45
1:B:619:PHE:C	1:B:621:THR:N	2.67	0.45
1:C:328:ASN:ND2	1:C:343:GLU:OE1	2.49	0.45
1:D:294:LYS:N	1:D:294:LYS:HD2	2.31	0.45
1:D:612:ALA:HB2	1:D:636:GLN:OE1	2.15	0.45
1:A:247:TYR:HB2	1:B:627:SER:CB	2.47	0.45
1:A:471:PHE:HA	1:A:474:ALA:HB3	1.98	0.45
1:B:328:ASN:OD1	1:B:343:GLU:HB3	2.15	0.45
1:B:501:HIS:O	1:B:505:SER:OG	2.33	0.45
1:C:384:ALA:CA	1:C:385:THR:HG22	2.35	0.45
1:A:293:TRP:CZ3	1:A:399:ARG:HG2	2.51	0.45
1:A:380:TRP:HB2	4:A:1007:PX6:H3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:TYR:O	1:B:220:VAL:HG22	2.17	0.45
1:B:406:VAL:O	1:B:410:LYS:N	2.47	0.45
1:B:467:THR:OG1	1:C:335:GLN:OE1	2.34	0.45
1:B:471:PHE:HA	1:B:474:ALA:HB3	1.98	0.45
1:D:216:TYR:O	1:D:220:VAL:HG22	2.17	0.45
1:D:310:PHE:CD1	1:D:310:PHE:N	2.83	0.45
1:D:460:LEU:HD13	1:D:555:GLN:HG2	1.99	0.45
1:A:458:GLN:HE21	1:A:459:PRO:HD2	1.81	0.45
1:A:556:ILE:HG22	1:A:560:ASN:OD1	2.17	0.45
1:A:561:ILE:O	1:A:565:THR:HG23	2.17	0.45
1:B:220:VAL:O	1:B:224:LEU:HG	2.17	0.45
1:B:328:ASN:ND2	1:B:343:GLU:OE1	2.49	0.45
1:C:328:ASN:OD1	1:C:343:GLU:HB3	2.15	0.45
1:C:591:SER:HA	1:C:594:ALA:CB	2.47	0.45
1:B:684:TYR:OH	1:C:679:ILE:HG12	2.16	0.45
1:D:334:PRO:HB2	1:D:337:LEU:HB2	1.98	0.45
1:D:400:GLU:OE1	1:D:400:GLU:N	2.36	0.45
1:D:556:ILE:HG22	1:D:560:ASN:OD1	2.17	0.45
1:A:220:VAL:O	1:A:224:LEU:HG	2.17	0.45
1:A:378:SER:HB3	1:A:387:SER:HA	1.98	0.45
1:B:224:LEU:O	1:B:228:LEU:HG	2.17	0.45
1:B:227:TYR:O	1:B:231:LEU:HB2	2.17	0.45
1:B:548:PHE:O	1:B:551:LEU:HB2	2.16	0.45
1:C:254:SER:O	1:C:257:PHE:N	2.39	0.45
1:C:678:ALA:O	1:C:682:ASP:N	2.32	0.45
1:D:220:VAL:O	1:D:224:LEU:HG	2.17	0.45
1:D:248:TYR:C	1:D:252:MET:HG2	2.36	0.45
1:D:601:ALA:HB1	1:D:605:PHE:CE2	2.52	0.45
1:A:227:TYR:O	1:A:231:LEU:HB2	2.17	0.45
1:A:430:ASN:ND2	1:A:435:LEU:HB3	2.27	0.45
1:A:467:THR:HG21	1:B:333:ILE:HG22	1.98	0.45
1:A:460:LEU:HD13	1:A:555:GLN:HG2	1.99	0.45
1:B:293:TRP:CZ3	1:B:399:ARG:HG2	2.51	0.45
1:B:591:SER:HA	1:B:594:ALA:CB	2.47	0.45
1:B:633:ILE:HA	1:B:633:ILE:HD12	1.62	0.45
1:C:378:SER:HB3	1:C:387:SER:HA	1.98	0.45
1:C:406:VAL:O	1:C:410:LYS:N	2.47	0.45
1:D:249:TYR:OH	1:D:430:ASN:HB3	2.17	0.45
1:D:319:PRO:HG3	1:D:426:PHE:CG	2.52	0.45
1:D:322:ARG:N	1:D:423:PHE:O	2.28	0.45
1:A:591:SER:HA	1:A:594:ALA:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:ALA:HB1	1:A:605:PHE:CE2	2.52	0.45
1:B:334:PRO:HB2	1:B:337:LEU:HB2	1.98	0.45
1:B:332:SER:HB2	1:B:344:CYS:HB3	1.98	0.45
1:B:548:PHE:CD2	1:B:552:ALA:HB2	2.52	0.45
1:C:216:TYR:O	1:C:220:VAL:HG22	2.17	0.45
1:C:347:VAL:HG12	1:C:348:TYR:N	2.32	0.45
1:D:378:SER:HB3	1:D:387:SER:HA	1.98	0.45
1:D:548:PHE:O	1:D:551:LEU:HB2	2.16	0.45
1:A:216:TYR:O	1:A:220:VAL:HG22	2.17	0.45
1:A:680:ILE:CG2	1:B:674:ASN:HB3	2.47	0.45
1:B:319:PRO:HG3	1:B:426:PHE:CG	2.52	0.45
1:C:249:TYR:OH	1:C:430:ASN:HB3	2.17	0.45
1:C:400:GLU:N	1:C:400:GLU:OE1	2.36	0.45
1:C:319:PRO:HG3	1:C:426:PHE:CG	2.52	0.45
1:C:548:PHE:CD2	1:C:552:ALA:HB2	2.52	0.45
1:A:224:LEU:O	1:A:228:LEU:HG	2.17	0.45
1:A:248:TYR:C	1:A:252:MET:HG2	2.36	0.45
1:A:501:HIS:O	1:A:505:SER:OG	2.33	0.45
3:B:1006:CHS:OH	3:B:1006:CHS:O	2.22	0.45
1:B:347:VAL:HG12	1:B:348:TYR:N	2.32	0.45
1:B:573:LEU:O	1:B:576:PHE:N	2.50	0.45
1:B:688:LYS:HA	1:B:691:LEU:HG	1.99	0.45
1:C:385:THR:O	1:C:385:THR:HG23	2.17	0.45
1:D:548:PHE:CD2	1:D:552:ALA:HB2	2.52	0.45
1:A:262:VAL:O	1:A:263:SER:OG	2.31	0.44
1:A:371:GLU:OE1	1:A:378:SER:HB3	2.18	0.44
1:B:456:GLN:NE2	4:B:1007:PX6:O1	2.50	0.44
1:B:561:ILE:O	1:B:565:THR:HG23	2.17	0.44
1:C:220:VAL:O	1:C:224:LEU:HG	2.17	0.44
1:C:688:LYS:HA	1:C:691:LEU:HG	2.00	0.44
1:D:591:SER:HA	1:D:594:ALA:CB	2.47	0.44
1:A:334:PRO:HB2	1:A:337:LEU:HB2	1.98	0.44
1:A:347:VAL:HG12	1:A:348:TYR:N	2.32	0.44
1:A:385:THR:O	1:A:385:THR:HG23	2.17	0.44
1:A:441:LEU:HD23	1:A:441:LEU:HA	1.74	0.44
1:A:436:PHE:CD1	1:A:460:LEU:HD23	2.53	0.44
1:B:460:LEU:HD13	1:B:555:GLN:HG2	1.99	0.44
1:B:556:ILE:HG22	1:B:560:ASN:OD1	2.17	0.44
1:C:227:TYR:O	1:C:231:LEU:HB2	2.17	0.44
1:C:248:TYR:CE2	1:D:452:ILE:HD12	2.52	0.44
1:C:279:PHE:CE1	1:C:443:VAL:HG21	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:SER:HB2	1:C:600:PHE:HE1	1.83	0.44
1:D:561:ILE:O	1:D:565:THR:HG23	2.16	0.44
1:D:573:LEU:O	1:D:576:PHE:N	2.50	0.44
1:A:319:PRO:HG3	1:A:426:PHE:CG	2.52	0.44
1:B:249:TYR:OH	1:B:430:ASN:HB3	2.17	0.44
1:C:377:SER:OG	1:C:378:SER:N	2.51	0.44
1:C:323:GLN:NE2	1:C:415:LEU:HB2	2.33	0.44
1:C:556:ILE:HG22	1:C:560:ASN:OD1	2.17	0.44
1:C:601:ALA:HB1	1:C:605:PHE:CE2	2.52	0.44
1:C:626:PHE:HA	1:C:632:CYS:SG	2.58	0.44
1:D:228:LEU:O	1:D:232:ILE:HD12	2.17	0.44
1:D:608:PHE:CZ	1:D:636:GLN:HB3	2.53	0.44
1:B:228:LEU:O	1:B:232:ILE:HD12	2.17	0.44
1:B:377:SER:OG	1:B:378:SER:N	2.51	0.44
1:B:279:PHE:CE1	1:B:443:VAL:HG21	2.53	0.44
1:B:667:PHE:O	1:B:671:ILE:N	2.31	0.44
1:C:355:ARG:HG2	1:C:368:TYR:CD1	2.53	0.44
1:C:471:PHE:HA	1:C:474:ALA:HB3	1.98	0.44
1:D:227:TYR:O	1:D:231:LEU:HB2	2.17	0.44
1:D:371:GLU:OE1	1:D:378:SER:HB3	2.17	0.44
1:A:228:LEU:O	1:A:232:ILE:HD12	2.17	0.44
1:A:536:LEU:O	1:A:540:GLU:HB3	2.17	0.44
1:A:573:LEU:HD12	1:B:606:ILE:HD13	1.84	0.44
1:A:573:LEU:O	1:A:576:PHE:N	2.50	0.44
1:B:378:SER:HB3	1:B:387:SER:HA	1.98	0.44
1:B:601:ALA:HB1	1:B:605:PHE:CE2	2.52	0.44
1:C:429:TYR:CE1	1:C:434:ASN:O	2.71	0.44
1:C:536:LEU:O	1:C:540:GLU:HB3	2.17	0.44
5:A:1009:PLM:H92	5:A:1009:PLM:H61	1.73	0.44
1:A:250:THR:OG1	1:B:622:GLN:HA	2.18	0.44
1:A:608:PHE:CZ	1:A:636:GLN:HB3	2.53	0.44
1:A:688:LYS:O	1:A:691:LEU:HG	2.18	0.44
1:B:295:MET:C	1:B:297:PRO:HD2	2.38	0.44
1:A:467:THR:HB	1:B:333:ILE:O	2.17	0.44
1:C:573:LEU:O	1:C:576:PHE:N	2.50	0.44
1:D:323:GLN:NE2	1:D:415:LEU:HB2	2.33	0.44
1:D:385:THR:O	1:D:385:THR:HG23	2.17	0.44
1:D:409:LEU:HD13	1:D:414:TRP:HD1	1.83	0.44
1:A:249:TYR:OH	1:A:430:ASN:HB3	2.17	0.44
4:B:1007:PX6:H46	4:B:1007:PX6:H53	1.65	0.44
1:B:429:TYR:CE1	1:B:434:ASN:O	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:LEU:O	1:B:540:GLU:HB3	2.17	0.44
1:C:228:LEU:O	1:C:232:ILE:HD12	2.17	0.44
1:C:460:LEU:HD13	1:C:555:GLN:HG2	1.99	0.44
1:C:608:PHE:CZ	1:C:636:GLN:HB3	2.53	0.44
1:A:627:SER:CB	1:D:247:TYR:HB2	2.47	0.44
1:D:325:ARG:NH2	1:D:355:ARG:HA	2.29	0.44
1:D:429:TYR:CE1	1:D:434:ASN:O	2.71	0.44
1:D:536:LEU:O	1:D:540:GLU:HB3	2.17	0.44
1:D:688:LYS:HA	1:D:691:LEU:HG	1.99	0.44
1:A:279:PHE:CE1	1:A:443:VAL:HG21	2.53	0.44
1:A:626:PHE:HA	1:A:632:CYS:SG	2.58	0.44
1:A:688:LYS:HA	1:A:691:LEU:HG	2.00	0.44
1:B:262:VAL:O	1:B:263:SER:OG	2.31	0.44
1:B:323:GLN:NE2	1:B:415:LEU:HB2	2.33	0.44
1:C:224:LEU:O	1:C:228:LEU:HG	2.17	0.44
1:D:295:MET:C	1:D:297:PRO:HD2	2.38	0.44
1:D:355:ARG:HG2	1:D:368:TYR:CD1	2.53	0.44
1:D:436:PHE:CD1	1:D:460:LEU:HD23	2.53	0.44
1:A:409:LEU:HD13	1:A:414:TRP:HD1	1.83	0.44
1:A:230:PHE:HE1	1:A:480:PHE:HB2	1.83	0.44
5:B:1009:PLM:H42	5:B:1009:PLM:H71	1.60	0.44
1:B:385:THR:HG23	1:B:385:THR:O	2.17	0.44
1:B:517:LEU:HA	1:B:561:ILE:HD11	2.00	0.44
1:B:597:LEU:O	1:B:601:ALA:HB2	2.18	0.44
1:C:295:MET:C	1:C:297:PRO:HD2	2.38	0.44
1:C:334:PRO:HB2	1:C:337:LEU:HB2	1.98	0.44
1:C:440:ARG:O	1:C:456:GLN:N	2.51	0.44
1:C:517:LEU:HA	1:C:561:ILE:HD11	2.00	0.44
1:D:224:LEU:O	1:D:228:LEU:HG	2.17	0.44
1:D:279:PHE:CE1	1:D:443:VAL:HG21	2.53	0.44
1:D:347:VAL:HG12	1:D:348:TYR:N	2.32	0.44
1:D:323:GLN:NE2	1:D:415:LEU:O	2.44	0.44
1:A:283:THR:HG1	1:A:284:GLU:H	1.63	0.43
1:A:355:ARG:HG2	1:A:368:TYR:CD1	2.53	0.43
1:A:323:GLN:NE2	1:A:415:LEU:HB2	2.33	0.43
1:A:440:ARG:O	1:A:456:GLN:N	2.51	0.43
1:A:548:PHE:CD2	1:A:552:ALA:HB2	2.52	0.43
1:B:296:GLN:N	1:B:297:PRO:HD2	2.33	0.43
1:B:688:LYS:O	1:B:691:LEU:HG	2.18	0.43
1:C:283:THR:HG1	1:C:284:GLU:H	1.65	0.43
1:C:296:GLN:N	1:C:297:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ILE:HG13	1:C:313:ASN:C	2.38	0.43
1:C:406:VAL:HG13	1:C:414:TRP:NE1	2.24	0.43
1:C:460:LEU:CD1	1:C:555:GLN:HE21	2.31	0.43
1:D:458:GLN:HE21	1:D:459:PRO:HD2	1.81	0.43
1:D:460:LEU:CD1	1:D:555:GLN:HE21	2.31	0.43
1:C:247:TYR:HE1	1:D:623:VAL:C	2.21	0.43
1:D:688:LYS:O	1:D:691:LEU:HG	2.18	0.43
1:A:597:LEU:O	1:A:601:ALA:HB2	2.18	0.43
1:B:355:ARG:HG2	1:B:368:TYR:CD1	2.53	0.43
1:B:441:LEU:HD23	1:B:441:LEU:HA	1.74	0.43
1:B:542:GLN:HB3	1:B:544:THR:HG22	2.00	0.43
1:A:570:TRP:NE1	1:B:606:ILE:HG12	2.33	0.43
1:C:325:ARG:NH2	1:C:355:ARG:HA	2.29	0.43
1:C:379:HIS:HB3	1:C:423:PHE:CE2	2.53	0.43
1:D:377:SER:OG	1:D:378:SER:N	2.51	0.43
1:D:633:ILE:HD12	1:D:633:ILE:HA	1.62	0.43
4:A:1007:PX6:H24	5:A:1010:PLM:HG2	2.00	0.43
1:A:429:TYR:CE1	1:A:434:ASN:O	2.71	0.43
1:B:283:THR:OG1	1:B:284:GLU:N	2.51	0.43
1:A:249:TYR:CD1	1:B:448:THR:HB	2.53	0.43
4:C:1007:PX6:H54	4:C:1007:PX6:H61	1.89	0.43
1:C:458:GLN:CG	1:C:556:ILE:HG12	2.49	0.43
1:D:379:HIS:HB3	1:D:423:PHE:CE2	2.54	0.43
1:D:462:LEU:HD12	1:D:463:ILE:N	2.33	0.43
1:D:471:PHE:HA	1:D:474:ALA:HB3	1.98	0.43
1:A:377:SER:OG	1:A:378:SER:N	2.51	0.43
1:B:427:SER:CB	1:B:438:VAL:HA	2.49	0.43
1:C:371:GLU:OE1	1:C:378:SER:HB3	2.18	0.43
1:C:399:ARG:HD3	1:C:399:ARG:HA	1.80	0.43
1:C:427:SER:CB	1:C:438:VAL:HA	2.49	0.43
1:C:688:LYS:O	1:C:691:LEU:HG	2.18	0.43
1:D:296:GLN:N	1:D:297:PRO:HD2	2.33	0.43
1:A:460:LEU:CD1	1:A:555:GLN:HE21	2.31	0.43
1:B:371:GLU:OE1	1:B:378:SER:HB3	2.17	0.43
1:B:440:ARG:O	1:B:456:GLN:N	2.51	0.43
1:B:462:LEU:HD12	1:B:463:ILE:N	2.33	0.43
1:B:482:PHE:HA	1:B:485:PHE:HB3	2.01	0.43
1:B:460:LEU:CD1	1:B:555:GLN:HE21	2.31	0.43
1:B:608:PHE:C	1:B:636:GLN:HE22	2.15	0.43
1:A:677:LEU:C	1:B:674:ASN:HD22	2.22	0.43
1:B:676:PHE:O	1:B:680:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:PHE:HE1	1:C:480:PHE:HB2	1.83	0.43
1:C:349:SER:OG	1:C:350:VAL:N	2.52	0.43
1:D:327:ARG:NH1	1:D:351:SER:O	2.30	0.43
1:D:517:LEU:HA	1:D:561:ILE:HD11	2.00	0.43
1:D:458:GLN:CG	1:D:556:ILE:HG12	2.49	0.43
1:A:283:THR:OG1	1:A:284:GLU:N	2.51	0.43
1:A:306:ARG:CD	1:A:308:PHE:HZ	2.32	0.43
1:A:359:GLY:HA2	1:A:366:TRP:NE1	2.34	0.43
1:B:264:LYS:HG2	1:B:264:LYS:O	2.19	0.43
1:B:479:ILE:HA	1:B:482:PHE:CE2	2.54	0.43
1:C:283:THR:OG1	1:C:284:GLU:N	2.51	0.43
1:C:542:GLN:HB3	1:C:544:THR:HG22	2.00	0.43
1:C:597:LEU:O	1:C:601:ALA:HB2	2.18	0.43
1:D:440:ARG:O	1:D:456:GLN:N	2.51	0.43
1:A:532:VAL:HG12	1:A:536:LEU:HD13	2.01	0.43
1:A:536:LEU:HD21	1:A:548:PHE:CD1	2.54	0.43
1:A:542:GLN:HB3	1:A:544:THR:HG22	2.00	0.43
1:A:532:VAL:HG11	1:A:551:LEU:HD11	2.00	0.43
1:B:349:SER:OG	1:B:350:VAL:N	2.52	0.43
1:C:436:PHE:CD1	1:C:460:LEU:HD23	2.53	0.43
1:D:536:LEU:HD21	1:D:548:PHE:CD1	2.54	0.43
1:D:599:GLY:O	1:D:602:ILE:HG22	2.19	0.43
1:D:626:PHE:HA	1:D:632:CYS:SG	2.58	0.43
1:D:618:VAL:HG13	1:D:656:LEU:HD11	2.00	0.43
1:A:228:LEU:O	1:A:231:LEU:HB3	2.19	0.43
1:A:295:MET:C	1:A:297:PRO:HD2	2.38	0.43
1:A:322:ARG:NH1	1:A:371:GLU:OE2	2.52	0.43
1:A:327:ARG:NH1	1:A:351:SER:O	2.30	0.43
1:A:321:ILE:N	1:A:393:LEU:O	2.49	0.43
1:A:517:LEU:HA	1:A:561:ILE:HD11	2.00	0.43
1:A:618:VAL:HG13	1:A:656:LEU:HD11	2.00	0.43
1:A:676:PHE:O	1:A:680:ILE:HG13	2.19	0.43
1:B:291:LEU:HD12	1:B:291:LEU:HA	1.87	0.43
1:B:436:PHE:CD1	1:B:460:LEU:HD23	2.53	0.43
1:A:566:VAL:HG21	1:B:617:LEU:HD21	2.00	0.43
1:C:462:LEU:HD12	1:C:463:ILE:N	2.34	0.43
1:C:633:ILE:HD12	1:C:633:ILE:HA	1.62	0.43
1:D:349:SER:OG	1:D:350:VAL:N	2.52	0.43
1:D:597:LEU:O	1:D:601:ALA:HB2	2.18	0.43
1:A:264:LYS:HG2	1:A:264:LYS:O	2.19	0.43
1:B:228:LEU:O	1:B:231:LEU:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:GLY:HA2	1:B:366:TRP:NE1	2.34	0.43
1:B:432:ASN:HA	1:C:332:SER:HB3	2.01	0.43
3:C:1005:CHS:HD22	3:C:1006:CHS:HD23	2.01	0.43
1:C:428:VAL:N	1:C:437:CYS:O	2.50	0.43
1:D:427:SER:CB	1:D:438:VAL:HA	2.49	0.43
1:A:249:TYR:HD1	1:B:448:THR:HB	1.84	0.43
1:A:379:HIS:HB3	1:A:423:PHE:CE2	2.53	0.43
1:A:560:ASN:O	1:A:564:VAL:HG23	2.19	0.43
1:B:605:PHE:HZ	5:B:1009:PLM:HG3	1.84	0.43
1:B:379:HIS:HB3	1:B:423:PHE:CE2	2.53	0.43
1:B:230:PHE:HE1	1:B:480:PHE:HB2	1.83	0.43
1:B:458:GLN:CG	1:B:556:ILE:HG12	2.49	0.43
1:B:578:ASN:N	1:B:578:ASN:OD1	2.52	0.43
1:B:626:PHE:HA	1:B:632:CYS:SG	2.58	0.43
5:C:1009:PLM:H42	5:C:1009:PLM:H71	1.59	0.43
1:C:536:LEU:HD21	1:C:548:PHE:CD1	2.54	0.43
1:C:676:PHE:O	1:C:680:ILE:HG13	2.19	0.43
1:A:605:PHE:CZ	5:A:1009:PLM:HG3	2.53	0.42
1:A:296:GLN:N	1:A:297:PRO:HD2	2.33	0.42
1:A:406:VAL:O	1:A:410:LYS:N	2.47	0.42
1:A:458:GLN:CG	1:A:556:ILE:HG12	2.49	0.42
1:A:479:ILE:HA	1:A:482:PHE:CE2	2.54	0.42
1:A:532:VAL:HG12	1:A:536:LEU:CD1	2.49	0.42
1:B:433:ILE:O	1:B:434:ASN:OD1	2.37	0.42
1:B:532:VAL:HG11	1:B:551:LEU:HD11	2.00	0.42
1:B:532:VAL:HG12	1:B:536:LEU:HD13	2.01	0.42
1:B:599:GLY:O	1:B:602:ILE:HG22	2.19	0.42
1:B:618:VAL:HG13	1:B:656:LEU:HD11	2.00	0.42
1:B:608:PHE:CZ	1:B:636:GLN:HB3	2.53	0.42
1:B:680:ILE:CG2	1:C:674:ASN:HB3	2.49	0.42
3:C:1005:CHS:HE23	5:D:1010:PLM:H61	2.01	0.42
1:C:458:GLN:HE21	1:C:459:PRO:HD2	1.81	0.42
1:C:560:ASN:O	1:C:564:VAL:HG23	2.19	0.42
1:D:283:THR:OG1	1:D:284:GLU:N	2.51	0.42
1:A:462:LEU:HD12	1:A:463:ILE:N	2.33	0.42
1:A:482:PHE:HA	1:A:485:PHE:HB3	2.01	0.42
1:A:557:GLN:O	1:A:561:ILE:HG22	2.19	0.42
1:B:309:ILE:HD11	1:B:314:LEU:C	2.28	0.42
5:C:1008:PLM:HF1	5:C:1008:PLM:HB2	2.01	0.42
1:C:599:GLY:O	1:C:602:ILE:HG22	2.19	0.42
1:C:618:VAL:HG13	1:C:656:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:TYR:CZ	1:D:430:ASN:HB3	2.54	0.42
1:D:409:LEU:HD13	1:D:414:TRP:CD1	2.54	0.42
1:D:560:ASN:O	1:D:564:VAL:HG23	2.19	0.42
1:A:349:SER:OG	1:A:350:VAL:N	2.52	0.42
1:A:409:LEU:HD13	1:A:414:TRP:CD1	2.54	0.42
1:A:667:PHE:O	1:A:671:ILE:N	2.31	0.42
1:B:409:LEU:HD13	1:B:414:TRP:CD1	2.54	0.42
1:B:460:LEU:HD21	1:B:462:LEU:HA	2.02	0.42
1:B:536:LEU:HD21	1:B:548:PHE:CD1	2.54	0.42
1:B:557:GLN:O	1:B:561:ILE:HG22	2.19	0.42
1:C:322:ARG:NH1	1:C:371:GLU:OE2	2.52	0.42
1:C:359:GLY:HA2	1:C:366:TRP:NE1	2.34	0.42
1:C:668:MET:O	1:C:672:LEU:N	2.33	0.42
1:D:322:ARG:NH1	1:D:371:GLU:OE2	2.52	0.42
1:D:359:GLY:HA2	1:D:366:TRP:NE1	2.34	0.42
1:D:416:ASP:OD1	1:D:419:THR:OG1	2.38	0.42
1:D:479:ILE:HA	1:D:482:PHE:CE2	2.54	0.42
1:D:532:VAL:HG12	1:D:536:LEU:HD13	2.01	0.42
1:A:427:SER:CB	1:A:438:VAL:HA	2.49	0.42
1:B:311:TYR:HB3	1:C:417:ARG:HH11	1.84	0.42
1:C:320:ARG:NH1	1:C:547:ASN:HB2	2.35	0.42
1:C:409:LEU:HD13	1:C:414:TRP:CD1	2.54	0.42
1:C:479:ILE:HA	1:C:482:PHE:CE2	2.54	0.42
1:D:321:ILE:N	1:D:393:LEU:O	2.49	0.42
1:D:433:ILE:O	1:D:434:ASN:OD1	2.37	0.42
1:D:532:VAL:HG12	1:D:536:LEU:CD1	2.49	0.42
1:A:433:ILE:O	1:A:434:ASN:OD1	2.37	0.42
1:A:623:VAL:HG13	1:A:626:PHE:HB2	2.02	0.42
1:A:651:GLU:OE1	1:D:271:LYS:NZ	2.50	0.42
1:C:228:LEU:O	1:C:231:LEU:HB3	2.19	0.42
1:C:237:LEU:HB3	1:C:241:MET:HE2	2.02	0.42
1:C:264:LYS:O	1:C:264:LYS:HG2	2.19	0.42
1:C:532:VAL:HG11	1:C:551:LEU:HD11	2.00	0.42
1:D:623:VAL:HG13	1:D:626:PHE:HB2	2.02	0.42
1:A:599:GLY:O	1:A:602:ILE:HG22	2.19	0.42
1:A:681:ASN:O	1:A:685:SER:N	2.36	0.42
1:B:247:TYR:HB2	1:C:627:SER:CB	2.50	0.42
1:B:320:ARG:NH1	1:B:547:ASN:HB2	2.35	0.42
1:B:560:ASN:O	1:B:564:VAL:HG23	2.19	0.42
1:C:416:ASP:OD1	1:C:419:THR:OG1	2.38	0.42
1:C:460:LEU:HD21	1:C:462:LEU:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:PHE:HA	1:C:485:PHE:HB3	2.01	0.42
1:C:604:PHE:CZ	1:C:608:PHE:CD1	3.08	0.42
1:D:341:ILE:HD13	1:D:344:CYS:SG	2.60	0.42
1:D:532:VAL:HG11	1:D:551:LEU:HD11	2.00	0.42
1:A:361:ARG:C	2:A:1002:NAG:C8	2.80	0.42
1:B:321:ILE:N	1:B:393:LEU:O	2.49	0.42
1:B:428:VAL:N	1:B:437:CYS:O	2.50	0.42
1:B:532:VAL:HG12	1:B:536:LEU:CD1	2.50	0.42
1:B:587:SER:HB2	1:C:600:PHE:CE1	2.54	0.42
5:C:1010:PLM:H71	5:C:1010:PLM:H42	1.56	0.42
1:C:532:VAL:HG12	1:C:536:LEU:HD13	2.01	0.42
1:C:557:GLN:O	1:C:561:ILE:HG22	2.19	0.42
1:D:228:LEU:O	1:D:231:LEU:HB3	2.19	0.42
1:D:320:ARG:NH1	1:D:547:ASN:HB2	2.35	0.42
1:D:230:PHE:HE1	1:D:480:PHE:HB2	1.83	0.42
1:D:676:PHE:O	1:D:680:ILE:HG13	2.19	0.42
5:A:1009:PLM:H42	5:A:1009:PLM:H71	1.60	0.42
1:A:269:ASN:OD1	1:A:271:LYS:N	2.53	0.42
1:A:323:GLN:OE1	1:A:415:LEU:HB2	2.20	0.42
5:B:1008:PLM:HB2	5:B:1008:PLM:HF1	2.02	0.42
1:B:383:ILE:CD1	1:B:446:PRO:HG3	2.50	0.42
1:B:323:GLN:OE1	1:B:415:LEU:HB2	2.20	0.42
1:B:604:PHE:CZ	1:B:608:PHE:CD1	3.08	0.42
1:C:323:GLN:OE1	1:C:415:LEU:HB2	2.20	0.42
1:B:577:ILE:CG1	1:C:602:ILE:HD13	2.49	0.42
1:C:623:VAL:HG13	1:C:626:PHE:HB2	2.02	0.42
1:C:628:THR:O	1:C:631:GLU:N	2.51	0.42
1:D:323:GLN:OE1	1:D:415:LEU:HB2	2.20	0.42
1:D:460:LEU:HD21	1:D:462:LEU:HA	2.02	0.42
1:A:460:LEU:HD21	1:A:462:LEU:HA	2.02	0.42
1:B:249:TYR:CZ	1:B:430:ASN:HB3	2.54	0.42
1:C:269:ASN:OD1	1:C:271:LYS:N	2.53	0.42
1:C:341:ILE:HD13	1:C:344:CYS:SG	2.60	0.42
1:C:249:TYR:CZ	1:C:430:ASN:HB3	2.54	0.42
1:C:605:PHE:CZ	5:C:1009:PLM:HG3	2.54	0.42
4:D:1007:PX6:H46	4:D:1007:PX6:H53	1.65	0.42
1:D:262:VAL:O	1:D:263:SER:OG	2.31	0.42
1:C:432:ASN:HA	1:D:332:SER:HB3	2.02	0.42
1:D:557:GLN:O	1:D:561:ILE:HG22	2.19	0.42
1:D:571:ILE:O	1:D:574:PHE:N	2.53	0.42
1:A:416:ASP:OD1	1:A:419:THR:OG1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:THR:HG23	1:B:335:GLN:HB3	2.02	0.42
1:A:605:PHE:O	1:A:609:LEU:N	2.35	0.42
1:B:408:SER:O	1:B:411:LYS:HB3	2.20	0.42
1:C:409:LEU:HD13	1:C:414:TRP:HD1	1.83	0.42
1:C:667:PHE:O	1:C:671:ILE:N	2.31	0.42
1:D:264:LYS:O	1:D:264:LYS:HG2	2.19	0.42
1:A:383:ILE:CD1	1:A:446:PRO:HG3	2.50	0.41
1:A:408:SER:O	1:A:411:LYS:HB3	2.20	0.41
1:A:633:ILE:HD12	1:A:633:ILE:HA	1.62	0.41
1:B:409:LEU:HD13	1:B:414:TRP:HD1	1.83	0.41
1:C:433:ILE:O	1:C:434:ASN:OD1	2.37	0.41
1:C:571:ILE:O	1:C:574:PHE:N	2.53	0.41
1:A:320:ARG:NH1	1:A:547:ASN:HB2	2.35	0.41
1:A:604:PHE:CZ	1:A:608:PHE:CD1	3.08	0.41
1:B:322:ARG:NH1	1:B:371:GLU:OE2	2.52	0.41
1:B:623:VAL:HG13	1:B:626:PHE:HB2	2.02	0.41
1:B:628:THR:O	1:B:631:GLU:N	2.51	0.41
1:C:532:VAL:HG12	1:C:536:LEU:CD1	2.50	0.41
1:C:550:HIS:O	1:C:553:TYR:HB3	2.20	0.41
1:B:247:TYR:HB2	1:C:627:SER:HB3	2.03	0.41
1:D:380:TRP:HB2	4:D:1007:PX6:H3	2.03	0.41
1:D:383:ILE:CD1	1:D:446:PRO:HG3	2.50	0.41
1:D:542:GLN:HB3	1:D:544:THR:HG22	2.00	0.41
1:D:604:PHE:CZ	1:D:608:PHE:CD1	3.08	0.41
1:A:249:TYR:CZ	1:A:430:ASN:HB3	2.54	0.41
1:A:341:ILE:HD13	1:A:344:CYS:SG	2.60	0.41
1:A:628:THR:O	1:A:631:GLU:N	2.51	0.41
1:A:680:ILE:HG21	1:B:674:ASN:HB3	2.02	0.41
1:B:327:ARG:NH1	1:B:351:SER:O	2.31	0.41
1:C:325:ARG:NH2	1:C:356:ALA:H	2.17	0.41
1:D:398:THR:CB	2:D:1001:NAG:O6	2.69	0.41
1:D:605:PHE:O	1:D:609:LEU:N	2.35	0.41
5:A:1008:PLM:HB2	5:A:1008:PLM:HF1	2.02	0.41
1:A:237:LEU:HB3	1:A:241:MET:HE2	2.03	0.41
1:A:292:TYR:HB3	1:A:310:PHE:HE1	1.85	0.41
1:B:269:ASN:OD1	1:B:271:LYS:N	2.53	0.41
1:B:292:TYR:HB3	1:B:310:PHE:HE1	1.86	0.41
1:B:380:TRP:HB2	4:B:1007:PX6:H3	2.02	0.41
1:B:416:ASP:OD1	1:B:419:THR:OG1	2.38	0.41
1:D:269:ASN:OD1	1:D:271:LYS:N	2.53	0.41
1:D:325:ARG:NH2	1:D:356:ALA:H	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:SER:OG	1:D:386:TYR:O	2.26	0.41
5:B:1009:PLM:H61	5:B:1009:PLM:H92	1.73	0.41
1:B:502:TYR:HB2	1:B:508:ASN:HB2	2.03	0.41
1:C:292:TYR:HB3	1:C:310:PHE:HE1	1.86	0.41
1:C:608:PHE:CD2	1:C:633:ILE:HD11	2.55	0.41
5:A:1010:PLM:H61	3:D:1005:CHS:HE23	2.02	0.41
1:D:237:LEU:HB3	1:D:241:MET:HE2	2.02	0.41
1:D:655:VAL:C	1:D:658:PRO:HD2	2.41	0.41
1:A:379:HIS:CG	1:A:380:TRP:N	2.88	0.41
1:A:423:PHE:HA	1:A:423:PHE:HD1	1.72	0.41
1:A:608:PHE:CD2	1:A:633:ILE:HD11	2.55	0.41
1:A:615:ALA:O	1:A:619:PHE:N	2.37	0.41
1:C:327:ARG:NH1	1:C:351:SER:O	2.30	0.41
1:C:461:LYS:O	1:C:461:LYS:HG3	2.21	0.41
1:D:461:LYS:O	1:D:461:LYS:HG3	2.21	0.41
4:B:1007:PX6:H61	4:B:1007:PX6:H54	1.89	0.41
1:B:461:LYS:O	1:B:461:LYS:HG3	2.21	0.41
1:B:643:ASP:OD1	1:B:643:ASP:C	2.59	0.41
1:C:383:ILE:CD1	1:C:446:PRO:HG3	2.50	0.41
1:C:321:ILE:N	1:C:393:LEU:O	2.49	0.41
1:C:466:VAL:HB	1:C:470:ASP:H	1.86	0.41
1:D:379:HIS:CG	1:D:380:TRP:N	2.88	0.41
1:D:482:PHE:HA	1:D:485:PHE:HB3	2.01	0.41
1:A:396:SER:OG	1:A:402:THR:HB	2.21	0.41
5:D:1008:PLM:HF1	5:D:1008:PLM:HB2	2.02	0.41
1:D:628:THR:O	1:D:631:GLU:N	2.51	0.41
1:A:642:GLY:HA2	1:D:641:LEU:HD21	2.02	0.41
1:A:325:ARG:HH21	1:A:356:ALA:N	2.18	0.41
1:A:335:GLN:HG2	1:A:336:ASP:N	2.36	0.41
1:A:325:ARG:NH2	1:A:356:ALA:H	2.17	0.41
1:B:237:LEU:O	1:B:241:MET:HG2	2.21	0.41
1:B:237:LEU:HB3	1:B:241:MET:HE2	2.03	0.41
1:B:550:HIS:O	1:B:553:TYR:HB3	2.20	0.41
1:C:237:LEU:O	1:C:241:MET:HG2	2.21	0.41
1:C:326:VAL:HG12	1:C:327:ARG:N	2.36	0.41
1:C:319:PRO:HG3	1:C:426:PHE:CD1	2.56	0.41
1:C:653:ASN:C	1:C:656:LEU:H	2.23	0.41
1:D:361:ARG:C	2:D:1002:NAG:C8	2.80	0.41
1:D:277:GLU:HA	1:D:280:TRP:HE3	1.86	0.41
1:D:550:HIS:O	1:D:553:TYR:HB3	2.20	0.41
1:D:653:ASN:C	1:D:656:LEU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLU:HA	1:A:280:TRP:HE3	1.86	0.41
1:A:550:HIS:O	1:A:553:TYR:HB3	2.20	0.41
1:A:570:TRP:CE3	1:B:613:GLN:OE1	2.74	0.41
1:B:455:TRP:CH2	1:C:651:GLU:CD	2.94	0.41
1:B:603:MET:HG3	1:B:604:PHE:N	2.36	0.41
1:B:608:PHE:CD2	1:B:633:ILE:HD11	2.56	0.41
1:B:586:LEU:HD21	1:B:691:LEU:HB3	2.03	0.41
1:C:502:TYR:HB2	1:C:508:ASN:HB2	2.03	0.41
1:D:221:LEU:O	1:D:225:VAL:HG23	2.21	0.41
1:D:399:ARG:HD3	1:D:399:ARG:HA	1.80	0.41
1:A:655:VAL:C	1:A:658:PRO:HD2	2.41	0.41
1:B:341:ILE:HD13	1:B:344:CYS:SG	2.60	0.41
1:B:357:PRO:O	1:B:366:TRP:HB3	2.21	0.41
1:C:251:ARG:O	1:C:254:SER:N	2.51	0.41
1:C:262:VAL:CG1	1:C:266:GLU:HB3	2.51	0.41
1:D:335:GLN:HG2	1:D:336:ASP:N	2.36	0.41
1:D:608:PHE:CD2	1:D:633:ILE:HD11	2.55	0.41
1:D:674:ASN:O	1:D:678:ALA:N	2.49	0.41
1:A:461:LYS:O	1:A:461:LYS:HG3	2.21	0.40
1:A:466:VAL:HB	1:A:470:ASP:H	1.86	0.40
1:A:502:TYR:HB2	1:A:508:ASN:HB2	2.03	0.40
1:B:308:PHE:CD1	1:B:308:PHE:N	2.86	0.40
1:B:326:VAL:HG12	1:B:327:ARG:N	2.36	0.40
1:A:311:TYR:HB3	1:B:417:ARG:NH1	2.35	0.40
1:C:309:ILE:HD11	1:C:315:LEU:CA	2.50	0.40
1:B:248:TYR:CE2	1:C:452:ILE:HD12	2.57	0.40
1:C:529:THR:O	1:C:533:GLU:HG3	2.21	0.40
1:D:529:THR:O	1:D:533:GLU:HG3	2.21	0.40
1:A:221:LEU:O	1:A:225:VAL:HG23	2.21	0.40
1:A:262:VAL:CG1	1:A:266:GLU:HB3	2.51	0.40
1:A:326:VAL:HG12	1:A:327:ARG:N	2.36	0.40
1:A:509:CYS:HA	1:A:512:VAL:HG22	2.03	0.40
1:A:529:THR:O	1:A:533:GLU:HG3	2.21	0.40
1:B:306:ARG:CG	1:B:308:PHE:HE1	2.30	0.40
1:B:503:PHE:C	1:B:505:SER:H	2.25	0.40
1:C:311:TYR:HB3	1:D:417:ARG:HH11	1.85	0.40
1:C:357:PRO:O	1:C:366:TRP:HB3	2.21	0.40
1:C:509:CYS:HA	1:C:512:VAL:HG22	2.03	0.40
1:C:643:ASP:C	1:C:643:ASP:OD1	2.59	0.40
1:D:254:SER:O	1:D:256:LEU:N	2.54	0.40
1:D:262:VAL:CG1	1:D:266:GLU:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:CYS:HA	1:D:512:VAL:HG22	2.04	0.40
1:D:586:LEU:HD21	1:D:691:LEU:HB3	2.03	0.40
1:A:237:LEU:O	1:A:241:MET:HG2	2.21	0.40
1:A:247:TYR:HB2	1:B:627:SER:HB3	2.03	0.40
1:B:254:SER:O	1:B:256:LEU:N	2.55	0.40
1:C:379:HIS:CG	1:C:380:TRP:N	2.89	0.40
1:C:396:SER:OG	1:C:402:THR:HB	2.21	0.40
1:D:310:PHE:C	1:D:312:GLU:H	2.25	0.40
1:D:357:PRO:O	1:D:366:TRP:HB3	2.21	0.40
1:A:549:GLU:O	1:A:552:ALA:N	2.54	0.40
1:B:221:LEU:O	1:B:225:VAL:HG23	2.21	0.40
1:B:262:VAL:CG1	1:B:266:GLU:HB3	2.51	0.40
1:B:306:ARG:CD	1:B:308:PHE:HZ	2.33	0.40
1:B:335:GLN:HG2	1:B:336:ASP:N	2.36	0.40
1:B:325:ARG:NH2	1:B:356:ALA:H	2.17	0.40
1:B:316:LEU:HD21	1:B:428:VAL:HA	2.04	0.40
1:B:655:VAL:C	1:B:658:PRO:HD2	2.41	0.40
1:C:503:PHE:C	1:C:505:SER:H	2.25	0.40
1:B:577:ILE:CG1	1:C:602:ILE:CD1	2.99	0.40
1:C:655:VAL:C	1:C:658:PRO:HD2	2.41	0.40
1:D:337:LEU:HD23	1:D:337:LEU:HA	1.85	0.40
1:D:408:SER:O	1:D:411:LYS:HB3	2.20	0.40
1:D:502:TYR:HB2	1:D:508:ASN:HB2	2.03	0.40
1:D:643:ASP:C	1:D:643:ASP:OD1	2.59	0.40
1:D:677:LEU:HA	1:D:677:LEU:HD23	1.88	0.40
1:A:643:ASP:C	1:A:643:ASP:OD1	2.59	0.40
1:A:653:ASN:C	1:A:656:LEU:H	2.23	0.40
1:A:682:ASP:CG	1:A:683:THR:N	2.75	0.40
1:A:586:LEU:HD21	1:A:691:LEU:HB3	2.03	0.40
1:B:319:PRO:HG3	1:B:426:PHE:CD1	2.56	0.40
1:B:379:HIS:CG	1:B:380:TRP:N	2.89	0.40
1:B:364:THR:HG23	1:B:392:TYR:CE1	2.57	0.40
1:B:653:ASN:C	1:B:656:LEU:H	2.23	0.40
1:C:254:SER:O	1:C:256:LEU:N	2.54	0.40
1:C:408:SER:O	1:C:411:LYS:HB3	2.20	0.40
1:C:438:VAL:HG22	1:C:458:GLN:O	2.22	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	471/968 (49%)	382 (81%)	87 (18%)	2 (0%)	39	80
1	B	471/968 (49%)	383 (81%)	86 (18%)	2 (0%)	39	80
1	C	471/968 (49%)	381 (81%)	88 (19%)	2 (0%)	39	80
1	D	471/968 (49%)	381 (81%)	87 (18%)	3 (1%)	30	74
All	All	1884/3872 (49%)	1527 (81%)	348 (18%)	9 (0%)	38	77

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	311	TYR
1	A	258	LEU
1	B	258	LEU
1	C	258	LEU
1	D	258	LEU
1	A	623	VAL
1	B	623	VAL
1	C	623	VAL
1	D	623	VAL

### 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	429/837 (51%)	426 (99%)	3 (1%)	88	94
1	B	429/837 (51%)	426 (99%)	3 (1%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	429/837 (51%)	426 (99%)	3 (1%)	88	94
1	D	429/837 (51%)	425 (99%)	4 (1%)	84	92
All	All	1716/3348 (51%)	1703 (99%)	13 (1%)	87	93

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	ILE
1	A	415	LEU
1	A	577	ILE
1	B	309	ILE
1	B	415	LEU
1	B	577	ILE
1	C	308	PHE
1	C	415	LEU
1	C	577	ILE
1	D	309	ILE
1	D	310	PHE
1	D	415	LEU
1	D	577	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	456	GLN
1	A	458	GLN
1	A	501	HIS
1	A	550	HIS
1	A	622	GLN
1	A	653	ASN
1	A	693	GLN
1	B	456	GLN
1	B	458	GLN
1	B	501	HIS
1	B	537	GLN
1	B	550	HIS
1	B	622	GLN
1	B	653	ASN
1	B	693	GLN
1	C	456	GLN

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Mol	Chain	Res	Type
1	C	458	GLN
1	C	501	HIS
1	C	537	GLN
1	C	550	HIS
1	C	613	GLN
1	C	622	GLN
1	C	653	ASN
1	C	693	GLN
1	D	456	GLN
1	D	458	GLN
1	D	501	HIS
1	D	537	GLN
1	D	550	HIS
1	D	622	GLN
1	D	653	ASN
1	D	693	GLN

### 5.3.3 RNA [i](#)

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 42 ligands modelled in this entry, 2 are monoatomic - leaving 40 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	1001	1	14,14,15	0.70	1 (7%)	15,19,21	0.81	1 (6%)
2	NAG	A	1002	1	14,14,15	0.39	0	15,19,21	1.15	2 (13%)
2	NAG	A	1003	1,2	14,14,15	0.48	0	15,19,21	1.15	2 (13%)
2	NAG	A	1004	2	14,14,15	0.38	0	15,19,21	1.16	2 (13%)
3	CHS	A	1005	-	12,15,15	0.21	0	12,19,19	0.58	0
3	CHS	A	1006	-	12,15,15	0.42	0	12,19,19	0.61	0
4	PX6	A	1007	-	39,39,43	1.42	5 (12%)	43,44,48	1.61	4 (9%)
5	PLM	A	1008	-	14,17,17	0.22	0	14,17,17	0.49	0
5	PLM	A	1009	-	14,17,17	0.17	0	14,17,17	0.69	0
5	PLM	A	1010	-	14,17,17	0.22	0	14,17,17	0.53	0
2	NAG	B	1001	1	14,14,15	0.60	0	15,19,21	0.79	1 (6%)
2	NAG	B	1002	1	14,14,15	0.38	0	15,19,21	1.15	2 (13%)
2	NAG	B	1003	1,2	14,14,15	0.49	0	15,19,21	1.14	2 (13%)
2	NAG	B	1004	2	14,14,15	0.39	0	15,19,21	1.16	2 (13%)
3	CHS	B	1005	-	12,15,15	0.22	0	12,19,19	0.58	0
3	CHS	B	1006	-	12,15,15	0.40	0	12,19,19	0.61	0
4	PX6	B	1007	-	39,39,43	1.42	5 (12%)	43,44,48	1.61	4 (9%)
5	PLM	B	1008	-	14,17,17	0.22	0	14,17,17	0.50	0
5	PLM	B	1009	-	14,17,17	0.17	0	14,17,17	0.68	0
5	PLM	B	1010	-	14,17,17	0.22	0	14,17,17	0.52	0
2	NAG	C	1001	1	14,14,15	0.54	0	15,19,21	0.66	1 (6%)
2	NAG	C	1002	1	14,14,15	0.38	0	15,19,21	1.15	2 (13%)
2	NAG	C	1003	1,2	14,14,15	0.45	0	15,19,21	1.13	2 (13%)
2	NAG	C	1004	2	14,14,15	0.40	0	15,19,21	1.17	2 (13%)
3	CHS	C	1005	-	12,15,15	0.21	0	12,19,19	0.58	0
3	CHS	C	1006	-	12,15,15	0.40	0	12,19,19	0.60	0
4	PX6	C	1007	-	39,39,43	1.42	5 (12%)	43,44,48	1.59	4 (9%)
5	PLM	C	1008	-	14,17,17	0.22	0	14,17,17	0.51	0
5	PLM	C	1009	-	14,17,17	0.17	0	14,17,17	0.67	0
5	PLM	C	1010	-	14,17,17	0.22	0	14,17,17	0.52	0
2	NAG	D	1001	1	14,14,15	0.88	1 (7%)	15,19,21	0.77	1 (6%)
2	NAG	D	1002	1	14,14,15	0.38	0	15,19,21	1.15	2 (13%)
2	NAG	D	1003	1	14,14,15	0.42	0	15,19,21	1.17	2 (13%)
2	NAG	D	1004	-	14,14,15	0.39	0	15,19,21	1.16	2 (13%)
3	CHS	D	1005	-	12,15,15	0.21	0	12,19,19	0.58	0
3	CHS	D	1006	-	12,15,15	0.40	0	12,19,19	0.62	0
4	PX6	D	1007	-	39,39,43	1.42	5 (12%)	43,44,48	1.61	4 (9%)
5	PLM	D	1008	-	14,17,17	0.22	0	14,17,17	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PLM	D	1009	-	14,17,17	0.17	0	14,17,17	0.68	0
5	PLM	D	1010	-	14,17,17	0.22	0	14,17,17	0.52	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	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1003	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1004	2	-	0/6/23/26	0/1/1/1
3	CHS	A	1005	-	-	0/10/20/20	0/1/1/1
3	CHS	A	1006	-	-	0/10/20/20	0/1/1/1
4	PX6	A	1007	-	-	0/41/41/45	0/0/0/0
5	PLM	A	1008	-	-	0/13/15/15	0/0/0/0
5	PLM	A	1009	-	-	0/13/15/15	0/0/0/0
5	PLM	A	1010	-	-	0/13/15/15	0/0/0/0
2	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1003	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1004	2	-	0/6/23/26	0/1/1/1
3	CHS	B	1005	-	-	0/10/20/20	0/1/1/1
3	CHS	B	1006	-	-	0/10/20/20	0/1/1/1
4	PX6	B	1007	-	-	0/41/41/45	0/0/0/0
5	PLM	B	1008	-	-	0/13/15/15	0/0/0/0
5	PLM	B	1009	-	-	0/13/15/15	0/0/0/0
5	PLM	B	1010	-	-	0/13/15/15	0/0/0/0
2	NAG	C	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1003	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1004	2	-	0/6/23/26	0/1/1/1
3	CHS	C	1005	-	-	0/10/20/20	0/1/1/1
3	CHS	C	1006	-	-	0/10/20/20	0/1/1/1
4	PX6	C	1007	-	-	0/41/41/45	0/0/0/0
5	PLM	C	1008	-	-	0/13/15/15	0/0/0/0
5	PLM	C	1009	-	-	0/13/15/15	0/0/0/0
5	PLM	C	1010	-	-	0/13/15/15	0/0/0/0
2	NAG	D	1001	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1002	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1003	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1004	-	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CHS	D	1005	-	-	0/10/20/20	0/1/1/1
3	CHS	D	1006	-	-	0/10/20/20	0/1/1/1
4	PX6	D	1007	-	-	0/41/41/45	0/0/0/0
5	PLM	D	1008	-	-	0/13/15/15	0/0/0/0
5	PLM	D	1009	-	-	0/13/15/15	0/0/0/0
5	PLM	D	1010	-	-	0/13/15/15	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1007	PX6	O7-C2	-2.91	1.38	1.46
4	D	1007	PX6	O7-C2	-2.89	1.38	1.46
4	C	1007	PX6	O7-C2	-2.88	1.38	1.46
4	B	1007	PX6	O7-C2	-2.86	1.38	1.46
4	D	1007	PX6	P1-O3	-2.36	1.45	1.55
4	C	1007	PX6	P1-O3	-2.36	1.45	1.55
4	B	1007	PX6	P1-O3	-2.36	1.45	1.55
4	A	1007	PX6	P1-O3	-2.34	1.45	1.55
2	A	1001	NAG	C1-C2	2.18	1.55	1.52
4	B	1007	PX6	O7-C20	2.26	1.40	1.34
4	A	1007	PX6	O7-C20	2.27	1.40	1.34
4	C	1007	PX6	O7-C20	2.27	1.40	1.34
4	D	1007	PX6	O7-C20	2.27	1.41	1.34
4	A	1007	PX6	O5-C4	2.94	1.42	1.33
4	D	1007	PX6	O5-C4	2.94	1.42	1.33
4	C	1007	PX6	O5-C4	2.94	1.42	1.33
4	B	1007	PX6	O5-C4	2.95	1.42	1.33
2	D	1001	NAG	C1-C2	3.08	1.56	1.52
4	C	1007	PX6	P1-O2	4.88	1.65	1.50
4	A	1007	PX6	P1-O2	4.89	1.65	1.50
4	D	1007	PX6	P1-O2	4.91	1.65	1.50
4	B	1007	PX6	P1-O2	4.91	1.65	1.50

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1007	PX6	O3-P1-O1	-2.59	100.26	110.60
4	D	1007	PX6	O3-P1-O1	-2.58	100.32	110.60
4	B	1007	PX6	O3-P1-O1	-2.58	100.32	110.60
4	C	1007	PX6	O3-P1-O1	-2.56	100.40	110.60
2	C	1003	NAG	C2-N2-C7	-2.42	119.96	123.11
2	A	1003	NAG	C2-N2-C7	-2.39	120.00	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1004	NAG	C2-N2-C7	-2.39	120.00	123.11
2	B	1003	NAG	C2-N2-C7	-2.38	120.00	123.11
2	C	1004	NAG	C2-N2-C7	-2.38	120.01	123.11
2	A	1004	NAG	C2-N2-C7	-2.37	120.02	123.11
2	C	1002	NAG	C2-N2-C7	-2.36	120.03	123.11
2	B	1004	NAG	C2-N2-C7	-2.36	120.04	123.11
2	D	1003	NAG	C2-N2-C7	-2.36	120.04	123.11
2	B	1002	NAG	C2-N2-C7	-2.35	120.05	123.11
2	D	1002	NAG	C2-N2-C7	-2.34	120.06	123.11
2	A	1002	NAG	C2-N2-C7	-2.34	120.06	123.11
2	C	1003	NAG	C8-C7-N2	2.02	119.98	116.10
2	B	1003	NAG	C8-C7-N2	2.04	120.01	116.10
2	C	1002	NAG	C8-C7-N2	2.05	120.02	116.10
2	B	1002	NAG	C8-C7-N2	2.05	120.03	116.10
2	D	1004	NAG	C8-C7-N2	2.05	120.03	116.10
2	D	1003	NAG	C8-C7-N2	2.05	120.03	116.10
2	B	1004	NAG	C8-C7-N2	2.05	120.03	116.10
2	A	1004	NAG	C8-C7-N2	2.06	120.04	116.10
2	A	1002	NAG	C8-C7-N2	2.06	120.04	116.10
2	D	1002	NAG	C8-C7-N2	2.06	120.04	116.10
2	A	1003	NAG	C8-C7-N2	2.06	120.05	116.10
2	C	1004	NAG	C8-C7-N2	2.07	120.07	116.10
2	C	1001	NAG	C1-O5-C5	2.09	115.21	112.14
2	D	1001	NAG	C1-O5-C5	2.52	115.85	112.14
2	B	1001	NAG	C1-O5-C5	2.58	115.93	112.14
2	A	1001	NAG	C1-O5-C5	2.69	116.09	112.14
4	A	1007	PX6	O7-C20-C21	2.73	117.27	111.53
4	C	1007	PX6	O7-C20-C21	2.76	117.33	111.53
4	A	1007	PX6	O5-C4-C5	2.85	120.61	111.85
4	C	1007	PX6	O5-C4-C5	2.86	120.64	111.85
4	B	1007	PX6	O5-C4-C5	2.86	120.66	111.85
4	D	1007	PX6	O5-C4-C5	2.88	120.70	111.85
4	B	1007	PX6	O7-C20-C21	2.93	117.70	111.53
4	D	1007	PX6	O7-C20-C21	2.95	117.74	111.53
4	C	1007	PX6	O5-C3-C2	8.00	130.30	108.70
4	A	1007	PX6	O5-C3-C2	8.04	130.40	108.70
4	D	1007	PX6	O5-C3-C2	8.05	130.42	108.70
4	B	1007	PX6	O5-C3-C2	8.09	130.54	108.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

33 monomers are involved in 101 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	NAG	8	0
2	A	1004	NAG	2	0
3	A	1005	CHS	2	0
3	A	1006	CHS	2	0
4	A	1007	PX6	3	0
5	A	1008	PLM	2	0
5	A	1009	PLM	4	0
5	A	1010	PLM	3	0
2	B	1002	NAG	8	0
2	B	1004	NAG	2	0
3	B	1005	CHS	3	0
3	B	1006	CHS	3	0
4	B	1007	PX6	6	0
5	B	1008	PLM	2	0
5	B	1009	PLM	3	0
5	B	1010	PLM	3	0
2	C	1002	NAG	8	0
2	C	1004	NAG	2	0
3	C	1005	CHS	4	0
3	C	1006	CHS	3	0
4	C	1007	PX6	4	0
5	C	1008	PLM	2	0
5	C	1009	PLM	4	0
5	C	1010	PLM	3	0
2	D	1001	NAG	6	0
2	D	1002	NAG	8	0
2	D	1004	NAG	2	0
3	D	1005	CHS	3	0
3	D	1006	CHS	2	0
4	D	1007	PX6	4	0
5	D	1008	PLM	2	0
5	D	1009	PLM	1	0
5	D	1010	PLM	3	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.