



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:52 PM UTC

PDB ID : 4BXS / pdb_00004bxs
Title : Crystal Structure of the Prothrombinase Complex from the Venom of Pseudonaja Textilis
Authors : Lechtenberg, B.C.; Murray-Rust, T.A.; Johnson, D.J.D.; Adams, T.E.; Krishnaswamy, S.; Camire, R.M.; Huntington, J.A.
Deposited on : 2013-07-15
Resolution : 3.32 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

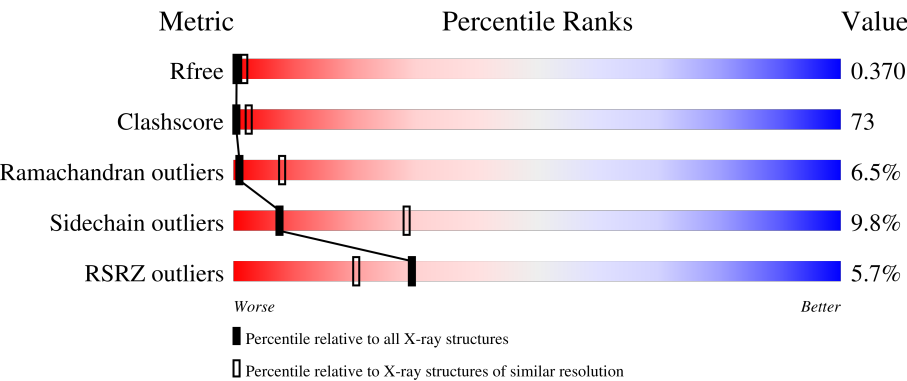
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	423	5% 35% 21% . 41%
2	V	1430	4% 27% 51% 10% . 12%
3	B	2	50% 50%
4	C	8	25% 62% 12%
5	D	2	100%

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Mol	Chain	Length	Quality of chain
5	E	2	 100%

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
5	NAG	E	1	X	-	-	-
6	NAG	V	1521	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11295 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called FACTOR X-LIKE PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1587	981	290	298	18			

- Molecule 2 is a protein called VENOM PROTHROMBIN ACTIVATOR PSEUTARIN-C NON-CATALYTIC SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	V	1262	Total	C	N	O	S	64	0	0
			9408	6020	1587	1766	35			

There are 3 discrepancies between the modelled and reference sequences:

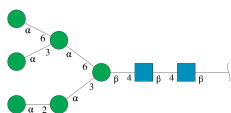
Chain	Residue	Modelled	Actual	Comment	Reference
V	50	LYS	GLU	conflict	UNP Q7SZN0
V	1287	LYS	SER	conflict	UNP Q7SZN0
V	1305	PHE	SER	conflict	UNP Q7SZN0

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



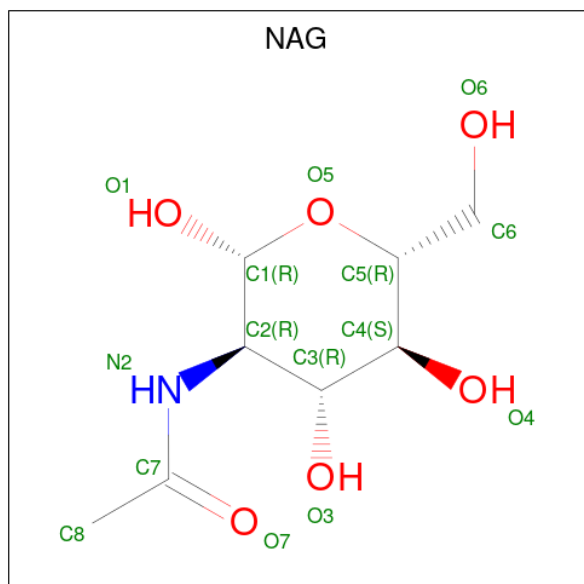
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	D	2	Total	C	N	O	0	0	0
			25	14	2	9			
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	V	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	V	2	Total 2	Ca 2	0	0

- Molecule 8 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	V	1	Total 1	Cu 1	0	0

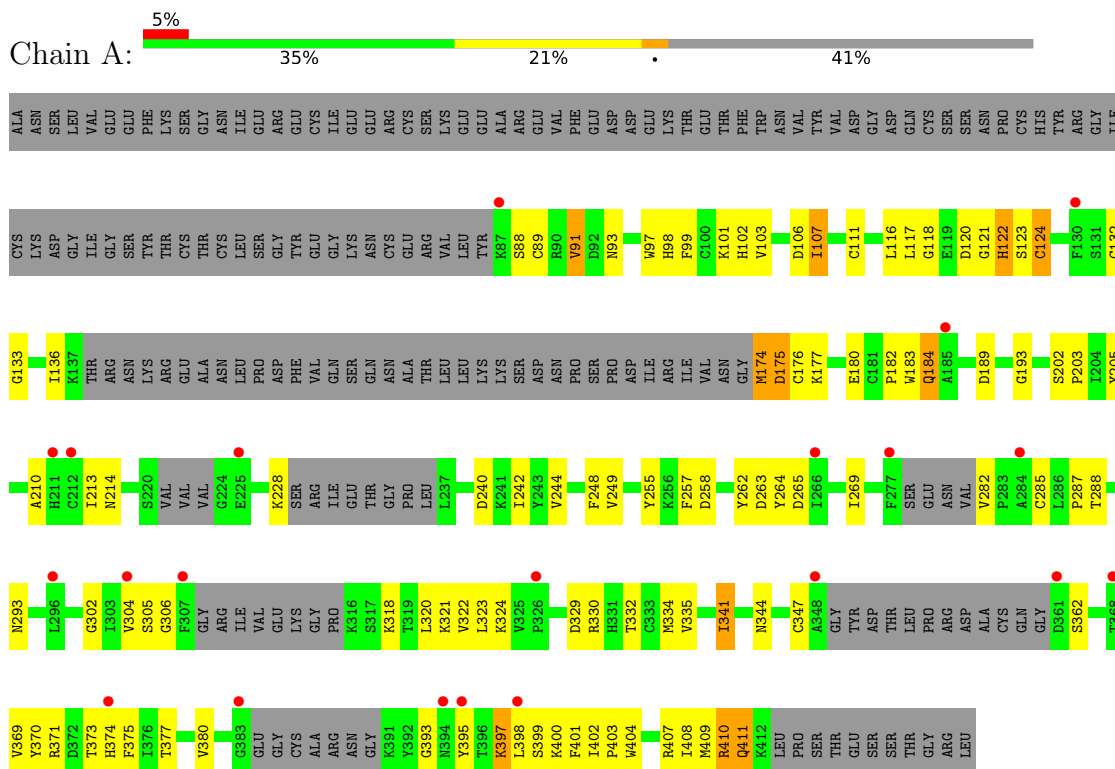
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	7	Total 7	O 7	0	0
9	V	105	Total 105	O 105	0	0

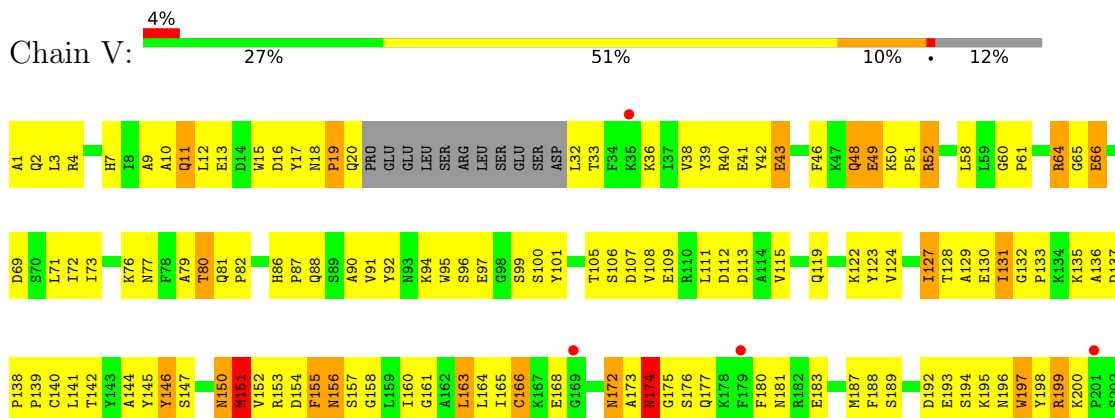
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

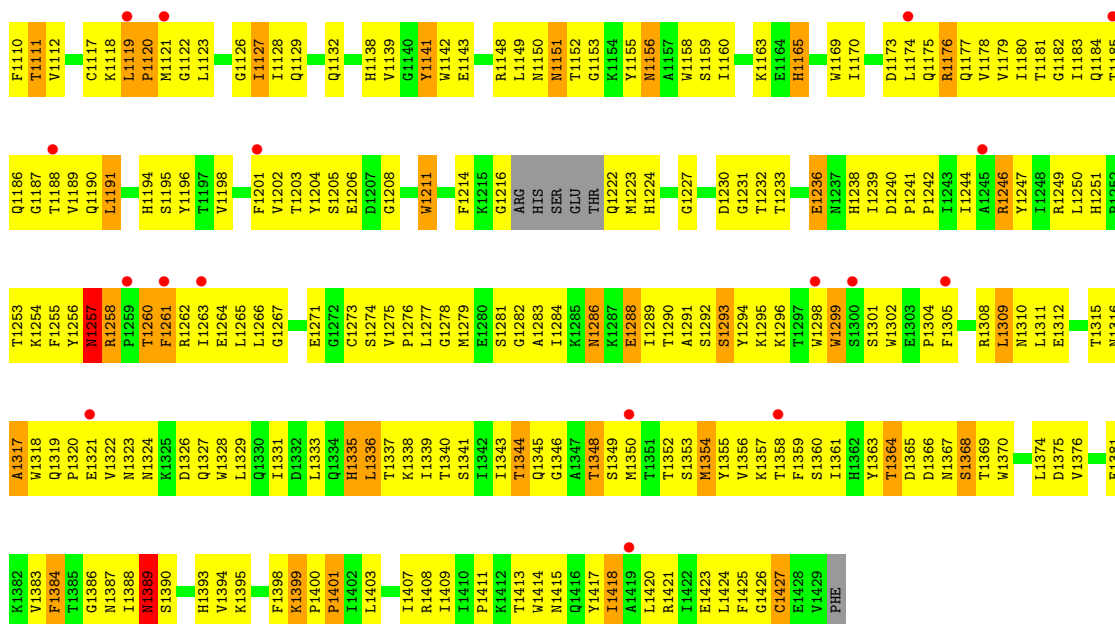
• Molecule 1: FACTOR X-LIKE PROTEASE



• Molecule 2: VENOM PROTHROMBIN ACTIVATOR PSEUTARIN-C NON-CATALYTIC SUB-UNIT



P1046	K1047	D1048	I1049	H1050	V1051	V1052	N1053	F1054	H1055	G1056	Q1057	T1058	F1059	E1062	R1063	R1064	E1065	D1066	N1067	Q1068	L1069	G1070	V1071	L1072	P1073	L1074	L1075	P1076	G1077	T1078	F1079	A1080	S1081	I1082	K1083	M1084	K1085	K1088	I1089	W1092	L1093	L1094	E1095	T1096	E1097	V1098	M1101	Q1102	E1103	R1104	G1105	M1106	Q1107	A1108	L1109																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
F986	D987	E988	E989	K990	S991	K992	Y993	F994	F995	L995	SER	ASP	LYS	THR	C1002	GLU	GLY	GLY	LYS	LEU	ILE	GLY	VAL	GLN	S1011	L1012	K948	K949	D950	F1015	T1016	A1017	I1018	M1019	G1020	G957	P958	I959	L960	K964	G965	N966	T967	D968	K969	K1032	D1033	N971	K906	K907	D908	D909	R977	E978	F979	N980	N981	G982	F983	N984	G1045																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
L854	L855	L858	L859	R860	L861	E862	R863	D864	D865	R866	L867	F871	K872	N873	L874	A875	S876	R877	F878	Y879	S880	L881	H882	A883	H884	G885	L886	L887	Y888	S891	E892	E893	G894	R895	S896	D898	D899	K900	S901	P902	F905	K906	K907	D908	D909	R977	E978	F979	N980	N981	G982	F983	N984	G1045																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
ASN	ARG	G793	H794	K795	R796	R797	Y798	Y799	R800	A801	A802	E803	E804	W807	D808	L874	A875	S876	R877	F878	Y879	S880	L881	H882	A883	H884	G885	L886	L887	Y888	S891	E892	E893	G894	R895	S896	D898	D899	K900	S901	P902	F905	K906	K907	D908	D909	R977	E978	F979	N980	N981	G982	F983	N984	G1045																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
GLN	GLN	LEU	MET	LYS	ALA	SER	MET	LEU	GLY	LEU	ARG	SER	PHE	LYS	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	THR	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ASP	ASP	ALA	LEU	HIS	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
E669	D670	D673	L674	F675	L676	F679	L680	P681	Q611	S544	A545	V546	D483	R484	D549	D550	P551	K552	F553	Y554	K555	S556	N557	V558	N559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R535	L536	F537	T538	V539	C540	S541	N542	H543	L544	K545	I546	T547	K548	L549	V550	D551	P552	K553	F554	G555	N556	V557	L558	M559	Y560	T561	L562	N563	G564	K565	A503	I433	L573	R574	F575	H576	Q577	V580	V581	Q582	K512	A513	D514	V515	E516	Q517	H518	A519	V520	F521	A522	N523	I524	V525	V526	P527	D528	P529	H529	S530	L531	T532	N533	G534	R5



- Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 50% 50%

NAG1
FUC2

- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 25% 62% 12%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6
MAN7
MAN8

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%

NAG1
NAG2

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 100%

NAG1
NAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	115.31Å 115.31Å 429.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.81 – 3.32 89.81 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.1 (89.81-3.32) 99.1 (89.81-3.32)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.298 , 0.368 0.289 , 0.370	Depositor DCC
R_{free} test set	2264 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	86.3	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 192.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	11295	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, CU, FUC, NAG, CA, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.28	0/1617	0.76	3/2210 (0.1%)
2	V	0.29	1/9671 (0.0%)	0.76	11/13230 (0.1%)
All	All	0.29	1/11288 (0.0%)	0.76	14/15440 (0.1%)

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
2	V	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	657	TYR	C-N	5.51	1.41	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	670	ASP	O-C-N	-15.44	102.94	123.01
2	V	670	ASP	CA-C-N	11.26	137.75	120.75
2	V	670	ASP	C-N-CA	11.26	137.75	120.75
2	V	1095	GLU	N-CA-C	11.14	122.66	107.73
2	V	657	TYR	O-C-N	-8.87	112.42	122.09
2	V	49	GLU	CB-CA-C	-6.64	108.92	116.63
2	V	662	GLU	N-CA-C	6.55	118.22	111.14
2	V	132	GLY	CA-C-N	6.54	126.04	119.24
2	V	132	GLY	C-N-CA	6.54	126.04	119.24
2	V	657	TYR	CA-C-N	6.46	135.28	121.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	657	TYR	C-N-CA	6.46	135.28	121.45
1	A	91	VAL	N-CA-C	5.25	111.83	106.21
1	A	249	VAL	CA-C-N	5.05	123.30	119.66
1	A	249	VAL	C-N-CA	5.05	123.30	119.66

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	V	657	TYR	Peptide
2	V	658	ASP	Peptide
2	V	668	GLU	Peptide
2	V	669	GLU	Peptide
2	V	670	ASP	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1587	0	1171	123	0
2	V	9408	0	8230	1388	0
3	B	24	0	22	4	0
4	C	94	0	79	11	0
5	D	25	0	21	0	0
5	E	28	0	25	3	0
6	V	14	0	13	3	0
7	V	2	0	0	0	0
8	V	1	0	0	0	0
9	A	7	0	0	0	0
9	V	105	0	0	21	0
All	All	11295	0	9561	1507	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 73.

All (1507) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:337:ALA:HB3	2:V:362:LYS:CD	1.25	1.60
2:V:337:ALA:CB	2:V:362:LYS:HD3	1.11	1.55
2:V:1205:SER:CB	2:V:1211:TRP:HB3	1.32	1.55
2:V:1094:LEU:HD23	2:V:1110:PHE:CD1	1.36	1.53
2:V:1309:LEU:HD12	2:V:1423:GLU:CB	1.33	1.52
2:V:1094:LEU:CD2	2:V:1110:PHE:CD1	2.00	1.43
2:V:3:LEU:HD11	2:V:72:ILE:CD1	1.57	1.34
2:V:172:ASN:ND2	2:V:176:SER:O	1.62	1.30
2:V:989:GLU:OE1	2:V:1011:SER:N	1.65	1.29
2:V:795:LYS:O	2:V:796:ARG:HG3	1.12	1.28
2:V:337:ALA:O	2:V:362:LYS:HD2	1.35	1.25
2:V:1126:GLY:O	2:V:1128:ILE:N	1.69	1.24
2:V:80:THR:CG2	2:V:198:TYR:OH	1.87	1.23
2:V:80:THR:HG21	2:V:198:TYR:OH	1.06	1.23
2:V:228:TRP:NE1	2:V:271:MET:HE3	1.50	1.22
2:V:1309:LEU:CD1	2:V:1423:GLU:HB3	1.70	1.21
2:V:1309:LEU:CD1	2:V:1423:GLU:CB	2.16	1.21
2:V:1185:THR:HG23	2:V:1261:PHE:CE1	1.74	1.21
2:V:1185:THR:CG2	2:V:1261:PHE:HE1	1.53	1.20
1:A:334:MET:O	2:V:512:LYS:HE3	1.37	1.20
2:V:48:GLN:O	2:V:48:GLN:NE2	1.74	1.19
2:V:828:LYS:NZ	2:V:988:GLU:OE1	1.74	1.18
2:V:1038:TRP:NE1	2:V:1084:MET:HG3	1.58	1.18
2:V:1159:SER:OG	2:V:1258:ARG:HD2	1.03	1.18
2:V:1118:LYS:NZ	2:V:1181:THR:O	1.76	1.17
1:A:176:CYS:HB2	1:A:322:VAL:CG2	1.75	1.17
2:V:1057:GLN:HE21	2:V:1057:GLN:HA	1.07	1.16
2:V:177:GLN:NE2	2:V:183:GLU:OE2	1.77	1.16
2:V:1304:PRO:HA	2:V:1318:TRP:CD1	1.82	1.15
2:V:1159:SER:OG	2:V:1258:ARG:CD	1.96	1.14
2:V:873:ASN:O	2:V:874:LEU:HD12	1.45	1.13
2:V:1339:ILE:HD13	2:V:1407:ILE:HD11	1.28	1.13
2:V:1036:VAL:HG13	2:V:1084:MET:HB2	1.13	1.12
2:V:1205:SER:CB	2:V:1211:TRP:CB	2.25	1.12
2:V:163:LEU:HD23	2:V:164:LEU:N	1.61	1.12
2:V:1174:LEU:HD13	2:V:1178:VAL:HG21	1.16	1.12
2:V:39:TYR:O	2:V:40:ARG:HG3	1.47	1.11
2:V:877:ARG:HG3	2:V:877:ARG:HH11	1.12	1.11
2:V:1038:TRP:HE1	2:V:1084:MET:HG3	1.00	1.11
2:V:1044:GLY:HA3	2:V:1048:ASP:OD2	1.48	1.11
1:A:107:ILE:HD12	1:A:107:ILE:O	1.50	1.11
1:A:334:MET:O	2:V:512:LYS:CE	1.98	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:199:ARG:HG2	2:V:199:ARG:HH11	0.97	1.11
2:V:1258:ARG:HG2	2:V:1258:ARG:HH11	1.04	1.11
2:V:680:ILE:H	2:V:681:PRO:CD	1.64	1.10
2:V:1204:TYR:O	2:V:1211:TRP:HB2	1.50	1.10
2:V:3:LEU:HD11	2:V:72:ILE:HD11	1.20	1.09
2:V:64:ARG:HH11	2:V:64:ARG:HG3	1.01	1.09
2:V:199:ARG:HH11	2:V:199:ARG:CG	1.66	1.09
2:V:1339:ILE:CD1	2:V:1407:ILE:HD11	1.83	1.08
2:V:795:LYS:O	2:V:796:ARG:CG	2.01	1.08
2:V:1185:THR:HG23	2:V:1261:PHE:HE1	0.91	1.08
2:V:1339:ILE:HD13	2:V:1407:ILE:CD1	1.83	1.08
2:V:432:ALA:HA	2:V:481:ALA:HB3	1.33	1.07
2:V:1094:LEU:HD21	2:V:1110:PHE:HB3	1.32	1.07
1:A:176:CYS:HB2	1:A:322:VAL:HG23	1.31	1.06
2:V:1399:LYS:CB	2:V:1400:PRO:HD3	1.84	1.06
2:V:1246:ARG:HG3	2:V:1246:ARG:NH1	1.62	1.06
2:V:527:ASN:HD21	2:V:557:ASN:CB	1.68	1.06
2:V:433:ILE:HD11	2:V:447:ALA:HB2	1.37	1.05
2:V:558:VAL:HG23	2:V:558:VAL:O	1.56	1.05
2:V:160:ILE:HD13	2:V:187:MET:HE2	1.34	1.05
2:V:432:ALA:HA	2:V:481:ALA:CB	1.87	1.05
2:V:1309:LEU:CD1	2:V:1423:GLU:HB2	1.83	1.05
2:V:1240:ASP:O	2:V:1242:PRO:HD3	1.57	1.05
2:V:86:HIS:CE1	2:V:1055:HIS:HE1	1.75	1.05
1:A:106:ASP:O	1:A:107:ILE:HG23	1.56	1.04
2:V:1291:ALA:HB2	2:V:1304:PRO:CB	1.86	1.04
2:V:337:ALA:CA	2:V:362:LYS:HD3	1.87	1.04
2:V:1291:ALA:HB2	2:V:1304:PRO:HB3	1.35	1.04
2:V:50:LYS:HG2	2:V:51:PRO:HD2	1.05	1.03
2:V:337:ALA:O	2:V:362:LYS:CD	2.05	1.03
2:V:228:TRP:HE1	2:V:271:MET:HE3	1.03	1.03
1:A:240:ASP:O	2:V:680:ILE:CB	2.06	1.03
2:V:1246:ARG:HH11	2:V:1246:ARG:CG	1.71	1.03
1:A:214:ASN:OD1	2:V:679:PHE:CZ	2.13	1.02
2:V:830:ILE:HG12	2:V:831:PHE:H	1.24	1.02
2:V:17:TYR:OH	2:V:36:LYS:NZ	1.93	1.02
2:V:1036:VAL:HG13	2:V:1084:MET:CB	1.90	1.01
2:V:1058:THR:OG1	2:V:1068:GLN:OE1	1.78	1.01
2:V:1309:LEU:HD12	2:V:1423:GLU:HB3	1.21	1.01
2:V:527:ASN:HD22	2:V:527:ASN:H	1.03	1.00
2:V:1296:LYS:HA	2:V:1301:SER:CB	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1159:SER:HG	2:V:1258:ARG:HD2	1.21	0.99
6:V:1521:NAG:H3	6:V:1521:NAG:H82	1.44	0.99
2:V:1057:GLN:HE21	2:V:1057:GLN:CA	1.75	0.99
2:V:1298:TRP:HZ3	2:V:1299:TRP:CH2	1.79	0.99
2:V:849:GLU:OE2	2:V:972:ARG:NH2	1.96	0.98
2:V:160:ILE:CD1	2:V:187:MET:HE2	1.91	0.98
2:V:1309:LEU:HD12	2:V:1423:GLU:HB2	1.00	0.98
2:V:3:LEU:CD1	2:V:72:ILE:CD1	2.41	0.98
2:V:1126:GLY:C	2:V:1128:ILE:H	1.72	0.98
2:V:50:LYS:CG	2:V:51:PRO:HD2	1.92	0.98
2:V:1174:LEU:HD13	2:V:1178:VAL:CG2	1.93	0.98
2:V:600:SER:O	2:V:602:HIS:N	1.96	0.98
2:V:390:GLY:HA3	2:V:563:ASN:O	1.63	0.97
2:V:1174:LEU:CD1	2:V:1178:VAL:HG21	1.93	0.97
2:V:1304:PRO:CA	2:V:1318:TRP:CD1	2.47	0.97
2:V:808:ASP:HB2	2:V:824:THR:O	1.64	0.97
2:V:602:HIS:HE1	2:V:634:TRP:CD1	1.83	0.97
2:V:1214:PHE:CZ	2:V:1239:ILE:HG23	2.00	0.97
2:V:1246:ARG:HG3	2:V:1246:ARG:HH11	0.81	0.97
2:V:449:GLU:HB3	2:V:450:PRO:HD2	1.44	0.96
1:A:88:SER:O	1:A:91:VAL:N	1.99	0.96
2:V:392:LEU:HD11	2:V:563:ASN:OD1	1.65	0.96
2:V:252:ASN:O	2:V:252:ASN:ND2	1.98	0.96
2:V:1186:GLN:OE1	2:V:1262:ARG:NE	1.98	0.96
2:V:258:THR:CG2	2:V:620:SER:HB3	1.96	0.95
2:V:1094:LEU:CD2	2:V:1110:PHE:HD1	1.55	0.95
2:V:64:ARG:HH11	2:V:64:ARG:CG	1.79	0.94
2:V:1151:ASN:HD22	2:V:1152:THR:N	1.65	0.94
2:V:1068:GLN:O	2:V:1069:LEU:HG	1.66	0.94
2:V:1322:VAL:O	2:V:1327:GLN:NE2	1.99	0.94
2:V:1036:VAL:CG1	2:V:1084:MET:HB2	1.97	0.94
2:V:432:ALA:O	2:V:446:LYS:NZ	1.99	0.94
2:V:808:ASP:HA	2:V:824:THR:O	1.67	0.94
2:V:1286:ASN:H	2:V:1286:ASN:ND2	1.65	0.94
2:V:1409:ILE:HD12	2:V:1409:ILE:O	1.66	0.94
1:A:106:ASP:O	1:A:107:ILE:CG2	2.16	0.93
2:V:348:TYR:HD2	2:V:646:ASN:HD22	1.13	0.93
2:V:42:TYR:HA	2:V:49:GLU:HA	1.49	0.93
2:V:1258:ARG:HG2	2:V:1258:ARG:NH1	1.78	0.92
2:V:210:PHE:HD2	2:V:215:LEU:HD12	1.34	0.92
1:A:330:ARG:HG2	1:A:334:MET:HE2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:11:GLN:HE21	2:V:40:ARG:HD2	1.31	0.92
2:V:108:VAL:HG21	2:V:1403:LEU:O	1.70	0.92
2:V:942:TYR:CD2	2:V:951:ILE:HD11	2.05	0.92
2:V:1185:THR:CG2	2:V:1261:PHE:CE1	2.41	0.92
2:V:3:LEU:HD11	2:V:72:ILE:HD13	1.52	0.92
2:V:1298:TRP:HZ3	2:V:1299:TRP:CZ3	1.87	0.91
2:V:199:ARG:HG2	2:V:199:ARG:NH1	1.74	0.91
2:V:331:GLU:OE2	2:V:413:SER:N	2.02	0.91
2:V:1298:TRP:CZ3	2:V:1299:TRP:CZ3	2.59	0.91
2:V:95:TRP:C	2:V:112:ASP:OD2	2.14	0.91
2:V:160:ILE:CD1	2:V:187:MET:CE	2.49	0.91
2:V:291:ALA:O	4:C:1:NAG:H61	1.71	0.91
1:A:410:ARG:HG2	1:A:410:ARG:HH11	1.34	0.91
1:A:213:ILE:HD13	1:A:242:ILE:HG21	1.53	0.90
2:V:1194:HIS:HB3	2:V:1231:GLY:HA3	1.53	0.90
1:A:408:ILE:O	1:A:411:GLN:HB2	1.71	0.90
2:V:803:GLU:OE2	2:V:834:TYR:OH	1.90	0.90
2:V:527:ASN:ND2	2:V:557:ASN:CB	2.35	0.90
2:V:558:VAL:O	2:V:558:VAL:CG2	2.17	0.90
2:V:1195:SER:HA	2:V:1256:TYR:O	1.72	0.90
1:A:98:HIS:HD2	1:A:375:PHE:HZ	1.13	0.90
2:V:242:VAL:CG1	2:V:259:ILE:HB	2.01	0.90
2:V:1278:GLY:HA2	2:V:1281:SER:OG	1.72	0.89
2:V:1156:ASN:HD22	2:V:1156:ASN:H	1.17	0.89
2:V:1107:GLN:O	2:V:1107:GLN:HG3	1.68	0.89
2:V:1204:TYR:O	2:V:1211:TRP:CB	2.19	0.89
2:V:1286:ASN:HB3	2:V:1305:PHE:HB2	1.54	0.89
2:V:155:PHE:CD1	2:V:156:ASN:N	2.41	0.89
1:A:175:ASP:HA	1:A:320:LEU:O	1.71	0.88
2:V:242:VAL:HG12	2:V:259:ILE:HB	1.52	0.88
2:V:348:TYR:CE2	2:V:646:ASN:HB2	2.08	0.88
2:V:3:LEU:CD1	2:V:72:ILE:HD11	2.02	0.88
2:V:153:ARG:NE	2:V:195:LYS:O	2.06	0.88
2:V:1329:LEU:HB3	2:V:1409:ILE:HD11	1.55	0.88
2:V:897:TYR:O	2:V:899:ASP:N	2.05	0.88
2:V:826:PHE:CD2	2:V:988:GLU:HG2	2.07	0.88
2:V:64:ARG:HG3	2:V:64:ARG:NH1	1.83	0.88
2:V:525:ASP:OD2	2:V:528:LYS:NZ	2.07	0.88
2:V:1315:THR:HG23	2:V:1315:THR:O	1.73	0.88
2:V:1374:LEU:HA	2:V:1381:GLU:HA	1.53	0.88
2:V:329:ALA:O	2:V:411:LEU:HB2	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:949:LYS:HG3	2:V:990:LYS:O	1.74	0.88
2:V:1042:ASN:OD1	2:V:1076:PRO:HA	1.74	0.88
2:V:606:SER:OG	2:V:611:GLN:OE1	1.90	0.88
2:V:301:ASP:OD1	2:V:302:CYS:N	2.07	0.87
2:V:364:TYR:CD2	2:V:526:GLU:HG3	2.09	0.87
2:V:1203:THR:CG2	2:V:1249:ARG:HB2	2.03	0.87
2:V:1355:TYR:CD1	2:V:1389:ASN:O	2.27	0.87
2:V:804:GLU:OE2	2:V:993:TYR:OH	1.91	0.87
2:V:1126:GLY:C	2:V:1128:ILE:N	2.25	0.87
2:V:86:HIS:CE1	2:V:1055:HIS:CE1	2.62	0.87
6:V:1521:NAG:H82	6:V:1521:NAG:C3	2.05	0.87
2:V:1291:ALA:CB	2:V:1304:PRO:HB3	2.04	0.87
2:V:911:ILE:CG2	2:V:915:GLY:HA3	2.05	0.87
2:V:882:HIS:HD2	2:V:895:ARG:HD2	1.39	0.87
2:V:258:THR:HB	2:V:620:SER:HB3	1.56	0.87
2:V:808:ASP:CB	2:V:824:THR:O	2.22	0.86
1:A:176:CYS:HB2	1:A:322:VAL:HG21	1.55	0.86
2:V:337:ALA:HB3	2:V:362:LYS:CG	2.05	0.86
2:V:680:ILE:H	2:V:681:PRO:HD2	1.39	0.86
2:V:808:ASP:CA	2:V:824:THR:O	2.23	0.86
2:V:1176:ARG:NH2	2:V:1178:VAL:HG11	1.90	0.86
2:V:525:ASP:OD1	2:V:558:VAL:HG12	1.75	0.86
2:V:674:ILE:O	2:V:675:PHE:HB2	1.76	0.86
2:V:249:LEU:HD11	2:V:271:MET:HE2	1.56	0.86
2:V:1032:LYS:O	2:V:1033:ASP:HB2	1.75	0.86
1:A:98:HIS:CD2	1:A:375:PHE:HZ	1.93	0.86
2:V:1040:LEU:C	2:V:1041:LEU:HD12	2.01	0.86
2:V:871:PHE:CG	2:V:881:LEU:HD13	2.11	0.85
2:V:131:ILE:C	2:V:131:ILE:HD12	2.01	0.85
2:V:1094:LEU:HD21	2:V:1110:PHE:CB	2.05	0.85
2:V:337:ALA:CB	2:V:362:LYS:CD	2.08	0.85
2:V:1016:PRO:O	2:V:1106:MET:N	2.09	0.85
2:V:891:SER:O	2:V:917:TYR:OH	1.94	0.85
2:V:1203:THR:CG2	2:V:1251:HIS:NE2	2.40	0.85
2:V:631:LEU:HD23	2:V:631:LEU:H	1.41	0.85
2:V:180:PHE:CD2	2:V:227:SER:CB	2.59	0.84
2:V:1094:LEU:CD2	2:V:1110:PHE:CG	2.60	0.84
2:V:174:ASN:ND2	2:V:174:ASN:H	1.74	0.84
2:V:1039:HIS:HD1	2:V:1081:SER:HG	1.17	0.84
1:A:409:MET:C	1:A:411:GLN:H	1.85	0.84
2:V:163:LEU:HD23	2:V:164:LEU:H	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:505:SER:C	2:V:508:GLY:HA2	2.02	0.84
2:V:626:VAL:HG23	2:V:626:VAL:O	1.77	0.84
2:V:877:ARG:HH11	2:V:877:ARG:CG	1.89	0.84
2:V:1298:TRP:CZ3	2:V:1299:TRP:CE3	2.65	0.84
2:V:258:THR:CB	2:V:620:SER:HB3	2.08	0.83
2:V:830:ILE:HG12	2:V:831:PHE:N	1.92	0.83
2:V:1189:VAL:HG22	2:V:1194:HIS:ND1	1.94	0.83
2:V:80:THR:CG2	2:V:198:TYR:HH	1.79	0.83
2:V:187:MET:HE3	2:V:189:SER:CB	2.09	0.83
2:V:1056:GLY:O	2:V:1057:GLN:NE2	2.12	0.83
2:V:400:VAL:O	2:V:401:ARG:HB2	1.77	0.83
2:V:432:ALA:O	2:V:446:LYS:CE	2.27	0.83
2:V:433:ILE:HD11	2:V:447:ALA:CB	2.09	0.83
2:V:604:PHE:HA	2:V:626:VAL:HG12	1.60	0.83
2:V:1399:LYS:CB	2:V:1400:PRO:CD	2.57	0.83
2:V:1345:GLN:HA	2:V:1387:ASN:HD21	1.44	0.82
2:V:894:GLY:O	2:V:895:ARG:HG3	1.79	0.82
2:V:1057:GLN:HA	2:V:1057:GLN:NE2	1.92	0.82
2:V:1289:ILE:CG2	2:V:1304:PRO:O	2.27	0.82
2:V:599:LEU:O	2:V:600:SER:OG	1.98	0.82
2:V:1017:ALA:HB2	2:V:1022:PRO:HB3	1.60	0.82
2:V:1044:GLY:HA3	2:V:1048:ASP:CG	2.04	0.82
1:A:398:LEU:HD23	1:A:398:LEU:O	1.80	0.82
2:V:230:LEU:HD12	2:V:230:LEU:N	1.94	0.82
2:V:1286:ASN:CB	2:V:1305:PHE:HB2	2.08	0.82
2:V:1039:HIS:ND1	2:V:1081:SER:OG	2.13	0.82
1:A:213:ILE:HD13	1:A:242:ILE:CG2	2.10	0.81
2:V:680:ILE:H	2:V:681:PRO:HD3	1.44	0.81
1:A:107:ILE:O	1:A:107:ILE:CD1	2.28	0.81
2:V:64:ARG:O	2:V:71:LEU:HD21	1.80	0.81
2:V:630:ASN:O	2:V:654:ASP:OD2	1.97	0.81
2:V:1286:ASN:H	2:V:1286:ASN:HD22	1.27	0.81
2:V:155:PHE:HD1	2:V:156:ASN:N	1.78	0.81
1:A:133:GLY:HA2	1:A:374:HIS:HB2	1.62	0.81
2:V:432:ALA:O	2:V:446:LYS:HE3	1.81	0.81
2:V:36:LYS:CE	2:V:193:GLU:OE2	2.30	0.80
2:V:336:TYR:O	2:V:338:PRO:HD3	1.81	0.80
1:A:214:ASN:OD1	2:V:679:PHE:CE2	2.34	0.80
2:V:1289:ILE:HG21	2:V:1304:PRO:O	1.82	0.80
2:V:1203:THR:HG22	2:V:1249:ARG:HB2	1.63	0.80
2:V:527:ASN:HD22	2:V:527:ASN:N	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1174:LEU:CD1	2:V:1178:VAL:CG2	2.55	0.79
2:V:254:TYR:CE2	2:V:607:LYS:HG2	2.18	0.79
2:V:367:ALA:HB2	2:V:531:TYR:OH	1.82	0.79
2:V:804:GLU:OE2	2:V:875:ALA:HB1	1.83	0.79
2:V:882:HIS:CD2	2:V:895:ARG:HD2	2.16	0.79
2:V:1288:GLU:N	2:V:1288:GLU:OE1	2.15	0.79
2:V:1289:ILE:CD1	2:V:1308:ARG:HH12	1.96	0.78
2:V:396:ILE:O	2:V:397:LYS:HG3	1.82	0.78
2:V:331:GLU:HG3	2:V:412:ALA:HA	1.63	0.78
2:V:640:GLY:HA3	2:V:644:MET:CE	2.14	0.78
2:V:1151:ASN:HD22	2:V:1151:ASN:C	1.86	0.78
1:A:118:GLY:HA3	1:A:123:SER:HB2	1.65	0.78
2:V:1230:ASP:OD2	2:V:1233:THR:HG23	1.84	0.78
2:V:228:TRP:HE1	2:V:271:MET:CE	1.91	0.78
2:V:1119:LEU:HD13	2:V:1119:LEU:H	1.47	0.78
2:V:1294:TYR:HB2	2:V:1302:TRP:O	1.85	0.77
1:A:103:VAL:CB	1:A:106:ASP:CB	2.63	0.77
2:V:982:PHE:CE2	2:V:984:MET:HB2	2.20	0.77
2:V:1211:TRP:CZ2	2:V:1249:ARG:CZ	2.68	0.77
2:V:150:ASN:HB3	2:V:154:ASP:OD1	1.85	0.77
2:V:348:TYR:HD2	2:V:646:ASN:ND2	1.82	0.77
2:V:888:TYR:CD2	2:V:893:GLU:HA	2.20	0.77
1:A:334:MET:O	2:V:512:LYS:HE2	1.85	0.77
2:V:602:HIS:CE1	2:V:634:TRP:CD1	2.72	0.77
2:V:1051:VAL:HG12	2:V:1071:VAL:HG13	1.66	0.77
2:V:1156:ASN:H	2:V:1156:ASN:ND2	1.78	0.77
2:V:1289:ILE:HD11	2:V:1308:ARG:HH12	1.49	0.76
2:V:831:PHE:O	2:V:832:ARG:CB	2.32	0.76
1:A:98:HIS:ND1	1:A:124:CYS:SG	2.59	0.76
1:A:98:HIS:HD2	1:A:375:PHE:CZ	2.01	0.76
2:V:800:ILE:HG22	2:V:801:ALA:N	1.98	0.76
2:V:1038:TRP:CD1	2:V:1084:MET:HG3	2.21	0.76
2:V:1094:LEU:HD21	2:V:1110:PHE:CD1	2.19	0.76
2:V:911:ILE:HG22	2:V:915:GLY:HA3	1.67	0.76
1:A:118:GLY:CA	1:A:123:SER:HB2	2.15	0.76
2:V:17:TYR:HB3	2:V:211:ALA:HB3	1.67	0.76
2:V:51:PRO:HG2	9:V:2011:HOH:O	1.84	0.76
2:V:240:PHE:HB2	2:V:261:LEU:CD2	2.16	0.76
2:V:151:MET:SD	2:V:151:MET:N	2.59	0.76
2:V:1051:VAL:CG1	2:V:1071:VAL:CG1	2.64	0.76
2:V:1279:MET:O	2:V:1308:ARG:HD2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1345:GLN:HA	2:V:1387:ASN:ND2	2.01	0.76
2:V:873:ASN:OD1	2:V:874:LEU:N	2.18	0.76
2:V:1059:PHE:CE1	2:V:1069:LEU:HD12	2.21	0.75
2:V:1286:ASN:HD22	2:V:1286:ASN:N	1.82	0.75
2:V:106:SER:HB3	2:V:1401:PRO:O	1.86	0.75
2:V:581:VAL:HG11	2:V:628:MET:HE2	1.68	0.75
2:V:594:ILE:O	2:V:596:PRO:HD3	1.87	0.75
2:V:831:PHE:O	2:V:832:ARG:HB2	1.83	0.75
2:V:1030:MET:HE1	2:V:1110:PHE:CD2	2.20	0.75
2:V:510:GLN:HG3	2:V:516:GLU:HB2	1.69	0.75
2:V:1017:ALA:HB2	2:V:1022:PRO:CB	2.16	0.75
2:V:1186:GLN:OE1	2:V:1262:ARG:NH2	2.18	0.75
2:V:1198:VAL:O	2:V:1227:GLY:HA3	1.87	0.75
2:V:1203:THR:HG23	2:V:1203:THR:O	1.87	0.75
2:V:640:GLY:HA3	2:V:644:MET:HE2	1.67	0.75
2:V:228:TRP:NE1	2:V:271:MET:CE	2.42	0.75
2:V:337:ALA:C	2:V:362:LYS:HD2	2.11	0.75
2:V:600:SER:C	2:V:602:HIS:H	1.92	0.75
2:V:359:PHE:HE1	2:V:553:PHE:HA	1.52	0.74
2:V:1341:SER:O	2:V:1425:PHE:HB2	1.87	0.74
2:V:809:TYR:OH	2:V:828:LYS:NZ	2.20	0.74
1:A:402:ILE:N	1:A:403:PRO:HD2	2.02	0.74
2:V:626:VAL:O	2:V:626:VAL:CG2	2.35	0.74
2:V:1176:ARG:NH2	2:V:1178:VAL:CG1	2.49	0.74
2:V:1196:TYR:HA	2:V:1260:THR:OG1	1.87	0.74
2:V:554:TYR:CE1	2:V:558:VAL:HG11	2.23	0.74
2:V:365:LYS:NZ	9:V:2051:HOH:O	2.18	0.74
2:V:808:ASP:HB3	2:V:825:THR:HA	1.70	0.74
2:V:230:LEU:CD2	2:V:242:VAL:HG11	2.17	0.74
2:V:863:VAL:HA	2:V:923:VAL:HG12	1.68	0.74
2:V:43:GLU:OE1	2:V:48:GLN:CG	2.35	0.74
2:V:1036:VAL:CG1	2:V:1084:MET:CB	2.63	0.74
2:V:452:GLN:OE1	2:V:452:GLN:HA	1.88	0.74
4:C:6:MAN:H62	4:C:8:MAN:H3	1.67	0.74
2:V:478:TYR:CD1	2:V:494:GLY:O	2.41	0.73
2:V:601:GLY:O	2:V:926:ARG:NH2	2.21	0.73
2:V:800:ILE:HD12	2:V:800:ILE:N	2.02	0.73
2:V:150:ASN:O	2:V:152:VAL:N	2.21	0.73
2:V:1038:TRP:NE1	2:V:1084:MET:CG	2.46	0.73
2:V:153:ARG:HH21	2:V:197:TRP:HA	1.53	0.73
2:V:387:LYS:O	2:V:388:GLU:CB	2.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:496:LEU:C	2:V:496:LEU:HD23	2.13	0.73
2:V:326:PHE:HD1	2:V:407:VAL:HG21	1.52	0.73
2:V:15:TRP:CG	2:V:58:LEU:HD21	2.23	0.73
2:V:41:GLU:OE2	2:V:50:LYS:HD2	1.89	0.73
2:V:1017:ALA:HB1	2:V:1022:PRO:N	2.04	0.73
2:V:1189:VAL:HG13	2:V:1194:HIS:ND1	2.04	0.73
2:V:897:TYR:C	2:V:899:ASP:H	1.95	0.73
2:V:1038:TRP:CD1	2:V:1084:MET:CG	2.71	0.73
2:V:12:LEU:HD21	2:V:198:TYR:OH	1.88	0.73
2:V:163:LEU:CD2	2:V:164:LEU:N	2.47	0.73
2:V:177:GLN:HE21	2:V:183:GLU:CD	1.97	0.73
2:V:254:TYR:HE2	2:V:607:LYS:HG2	1.53	0.73
2:V:934:GLU:HG3	2:V:1062:GLU:HG2	1.71	0.73
2:V:36:LYS:HE3	2:V:193:GLU:OE2	1.89	0.73
2:V:1345:GLN:HB3	2:V:1421:ARG:HB2	1.70	0.73
2:V:1289:ILE:HD11	2:V:1308:ARG:NH1	2.03	0.72
2:V:1294:TYR:HB3	2:V:1304:PRO:HD3	1.70	0.72
2:V:445:GLY:HA3	2:V:454:TYR:CE2	2.24	0.72
2:V:1053:ASN:ND2	2:V:1097:GLU:OE2	2.22	0.72
2:V:1156:ASN:OD1	2:V:1188:THR:OG1	2.06	0.72
2:V:212:ASN:ND2	4:C:1:NAG:O6	2.23	0.72
2:V:680:ILE:N	2:V:681:PRO:CD	2.41	0.72
2:V:982:PHE:CE2	2:V:984:MET:CB	2.73	0.72
2:V:1169:TRP:HB3	2:V:1251:HIS:HD1	1.55	0.72
2:V:1223:MET:HG3	2:V:1224:HIS:CD2	2.25	0.72
2:V:1299:TRP:CD1	2:V:1299:TRP:H	2.08	0.72
6:V:1521:NAG:C3	6:V:1521:NAG:C8	2.64	0.72
2:V:348:TYR:CD2	2:V:646:ASN:HB2	2.24	0.72
2:V:830:ILE:CG1	2:V:831:PHE:H	2.02	0.72
2:V:894:GLY:O	2:V:895:ARG:CG	2.38	0.72
1:A:409:MET:O	1:A:411:GLN:N	2.23	0.71
2:V:337:ALA:HB3	2:V:362:LYS:CE	2.18	0.71
2:V:888:TYR:HB3	2:V:921:TRP:CD1	2.25	0.71
2:V:1139:VAL:H	2:V:1160:ILE:HA	1.55	0.71
2:V:261:LEU:HD23	2:V:261:LEU:H	1.54	0.71
2:V:86:HIS:HE1	2:V:1055:HIS:CE1	2.05	0.71
5:E:2:NAG:O7	5:E:2:NAG:H3	1.89	0.71
2:V:174:ASN:H	2:V:174:ASN:HD22	1.37	0.71
2:V:486:ARG:HG3	2:V:528:LYS:O	1.90	0.71
2:V:137:ASP:HB3	2:V:141:LEU:HD21	1.73	0.71
2:V:258:THR:HB	2:V:620:SER:CB	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:150:ASN:C	2:V:151:MET:SD	2.73	0.71
2:V:1142:TRP:CZ3	2:V:1188:THR:HG21	2.25	0.71
2:V:1203:THR:HG21	2:V:1251:HIS:NE2	2.06	0.71
2:V:326:PHE:CD1	2:V:407:VAL:HG21	2.25	0.71
2:V:337:ALA:C	2:V:362:LYS:CD	2.64	0.71
2:V:527:ASN:H	2:V:527:ASN:ND2	1.81	0.71
2:V:475:THR:O	2:V:476:LYS:HG3	1.91	0.71
2:V:1316:ASN:O	2:V:1317:ALA:HB2	1.89	0.71
2:V:877:ARG:HG3	2:V:877:ARG:NH1	1.93	0.71
2:V:1177:GLN:HE21	2:V:1206:GLU:CB	2.03	0.71
2:V:1273:CYS:SG	2:V:1427:CYS:N	2.63	0.71
2:V:1316:ASN:O	2:V:1317:ALA:CB	2.37	0.71
2:V:43:GLU:HB2	2:V:49:GLU:O	1.90	0.71
2:V:1289:ILE:CD1	2:V:1308:ARG:NH1	2.53	0.71
2:V:174:ASN:HD22	2:V:174:ASN:N	1.88	0.70
2:V:1152:THR:HG22	2:V:1153:GLY:N	2.05	0.70
2:V:1304:PRO:HA	2:V:1318:TRP:HD1	1.53	0.70
1:A:120:ASP:OD1	1:A:121:GLY:N	2.24	0.70
2:V:245:ASN:O	2:V:247:GLN:HG2	1.91	0.70
2:V:949:LYS:CG	2:V:990:LYS:O	2.39	0.70
2:V:165:ILE:HG22	2:V:165:ILE:O	1.90	0.70
2:V:1304:PRO:HB3	2:V:1318:TRP:NE1	2.06	0.70
2:V:922:GLN:O	2:V:924:PRO:HD3	1.91	0.70
2:V:449:GLU:O	2:V:452:GLN:HB2	1.91	0.70
2:V:1186:GLN:OE1	2:V:1262:ARG:CZ	2.39	0.70
1:A:106:ASP:C	1:A:107:ILE:HG23	2.17	0.70
2:V:271:MET:HG2	2:V:272:SER:H	1.56	0.70
2:V:372:TYR:CD2	2:V:377:PHE:HD1	2.08	0.70
2:V:1123:LEU:HB2	2:V:1264:GLU:HG3	1.72	0.70
2:V:43:GLU:OE1	2:V:48:GLN:HG3	1.92	0.69
2:V:348:TYR:C	2:V:350:ALA:H	2.00	0.69
2:V:526:GLU:OE1	2:V:526:GLU:HA	1.92	0.69
2:V:1291:ALA:CB	2:V:1304:PRO:CB	2.64	0.69
2:V:1022:PRO:O	2:V:1023:TYR:HB2	1.92	0.69
2:V:445:GLY:HA3	2:V:454:TYR:CZ	2.27	0.69
2:V:1156:ASN:HD21	2:V:1188:THR:HG21	1.57	0.69
2:V:199:ARG:CG	2:V:199:ARG:NH1	2.38	0.69
2:V:230:LEU:HD23	2:V:242:VAL:HG11	1.74	0.69
2:V:1304:PRO:CA	2:V:1318:TRP:HD1	1.99	0.69
2:V:1311:LEU:HD23	2:V:1311:LEU:O	1.92	0.69
2:V:480:SER:OG	2:V:487:ASP:OD2	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1186:GLN:CD	2:V:1262:ARG:HE	2.01	0.69
2:V:163:LEU:HD23	2:V:163:LEU:C	2.18	0.69
2:V:39:TYR:O	2:V:40:ARG:CG	2.36	0.69
2:V:641:SER:C	2:V:643:GLU:H	2.00	0.69
2:V:1094:LEU:HD22	2:V:1110:PHE:CD1	2.22	0.69
2:V:1265:LEU:O	2:V:1266:LEU:HD23	1.93	0.69
2:V:1291:ALA:HB3	2:V:1304:PRO:HG3	1.74	0.69
2:V:11:GLN:NE2	2:V:40:ARG:HD2	2.06	0.69
2:V:1034:GLU:O	2:V:1034:GLU:HG3	1.91	0.69
2:V:128:THR:HG22	2:V:129:ALA:N	2.07	0.68
2:V:1187:GLY:O	2:V:1231:GLY:O	2.11	0.68
2:V:1298:TRP:CZ3	2:V:1299:TRP:CD2	2.81	0.68
2:V:593:GLU:HB3	2:V:1046:PRO:HB2	1.76	0.68
2:V:803:GLU:CD	2:V:834:TYR:HH	1.98	0.68
2:V:1216:GLY:H	2:V:1222:GLN:HA	1.58	0.68
2:V:285:VAL:HB	2:V:288:HIS:HD2	1.58	0.68
2:V:1173:ASP:OD1	2:V:1175:GLN:N	2.23	0.68
1:A:344:ASN:O	1:A:397:LYS:HB3	1.92	0.68
2:V:80:THR:HG21	2:V:198:TYR:HH	0.83	0.68
2:V:12:LEU:HA	2:V:36:LYS:O	1.93	0.68
2:V:240:PHE:HB2	2:V:261:LEU:HD21	1.76	0.68
2:V:1205:SER:CB	2:V:1211:TRP:CE3	2.77	0.68
2:V:615:ASN:ND2	2:V:1076:PRO:HD2	2.08	0.68
2:V:1211:TRP:HZ2	2:V:1249:ARG:CZ	2.05	0.68
1:A:335:VAL:HA	2:V:512:LYS:HE2	1.75	0.68
2:V:1339:ILE:HD11	2:V:1407:ILE:HD11	1.75	0.67
1:A:370:TYR:CD2	1:A:371:ARG:HG3	2.29	0.67
1:A:410:ARG:HG2	1:A:410:ARG:NH1	2.09	0.67
2:V:808:ASP:CB	2:V:825:THR:HA	2.25	0.67
2:V:977:ARG:HB3	2:V:1036:VAL:HG23	1.76	0.67
2:V:575:PHE:CD2	2:V:628:MET:HE3	2.29	0.67
2:V:160:ILE:HD11	2:V:187:MET:CE	2.24	0.67
2:V:808:ASP:HB3	2:V:825:THR:OG1	1.95	0.67
2:V:1176:ARG:HH21	2:V:1178:VAL:CG1	2.07	0.67
1:A:213:ILE:HD12	1:A:244:VAL:HG22	1.75	0.67
2:V:1021:ILE:HD12	2:V:1025:LEU:CD1	2.24	0.67
2:V:1094:LEU:HD21	2:V:1110:PHE:CG	2.29	0.67
2:V:1198:VAL:O	2:V:1227:GLY:CA	2.43	0.67
2:V:360:ILE:HG23	2:V:539:TYR:HB2	1.76	0.67
2:V:422:GLY:HA3	2:V:476:LYS:HD3	1.77	0.67
2:V:924:PRO:HG2	2:V:926:ARG:HH11	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PHE:CZ	1:A:287:PRO:HA	2.29	0.67
2:V:1094:LEU:HD23	2:V:1110:PHE:HD1	0.73	0.67
2:V:230:LEU:HD12	2:V:230:LEU:H	1.59	0.67
2:V:606:SER:O	2:V:607:LYS:C	2.38	0.67
2:V:1298:TRP:HZ3	2:V:1299:TRP:CZ2	2.12	0.67
2:V:1388:ILE:O	2:V:1389:ASN:HB3	1.93	0.67
1:A:304:VAL:O	1:A:306:GLY:N	2.28	0.67
2:V:17:TYR:CD2	2:V:206:THR:HG21	2.30	0.67
2:V:1094:LEU:HD23	2:V:1110:PHE:CE1	2.23	0.66
2:V:128:THR:HG22	2:V:130:GLU:H	1.59	0.66
2:V:210:PHE:CD2	2:V:215:LEU:HD12	2.25	0.66
2:V:256:VAL:O	2:V:257:SER:HB2	1.95	0.66
2:V:562:LEU:HD13	2:V:650:LEU:HD23	1.77	0.66
2:V:228:TRP:HB3	2:V:230:LEU:HD11	1.76	0.66
2:V:381:THR:O	2:V:381:THR:HG22	1.94	0.66
2:V:577:GLN:NE2	2:V:631:LEU:HB3	2.10	0.66
2:V:911:ILE:HD11	2:V:917:TYR:HB2	1.78	0.66
2:V:981:LEU:HD22	2:V:1018:ILE:HD11	1.77	0.66
2:V:1198:VAL:O	2:V:1227:GLY:N	2.27	0.66
2:V:1198:VAL:C	2:V:1227:GLY:HA3	2.20	0.66
2:V:17:TYR:CE2	2:V:204:GLN:CB	2.79	0.66
2:V:1126:GLY:O	2:V:1127:ILE:C	2.35	0.66
2:V:1398:PHE:O	2:V:1399:LYS:C	2.38	0.66
2:V:94:LYS:HB2	9:V:2017:HOH:O	1.96	0.66
2:V:396:ILE:O	2:V:397:LYS:CG	2.43	0.66
2:V:883:ALA:HB1	2:V:886:LEU:HD12	1.78	0.66
2:V:1194:HIS:HB3	2:V:1231:GLY:CA	2.26	0.66
2:V:943:SER:OG	2:V:955:LEU:HD23	1.95	0.65
2:V:1190:GLN:O	2:V:1191:LEU:CB	2.44	0.65
2:V:153:ARG:O	9:V:2031:HOH:O	2.12	0.65
2:V:155:PHE:O	2:V:158:GLY:N	2.28	0.65
2:V:1203:THR:HG22	2:V:1251:HIS:NE2	2.10	0.65
2:V:86:HIS:O	2:V:145:TYR:HA	1.96	0.65
2:V:673:ASP:OD1	2:V:674:ILE:N	2.29	0.65
2:V:1203:THR:HG23	2:V:1249:ARG:HB2	1.77	0.65
2:V:294:TYR:HE1	2:V:296:TYR:CE1	2.14	0.65
2:V:430:GLU:OE2	2:V:434:TYR:OH	2.08	0.65
2:V:396:ILE:HG22	2:V:397:LYS:N	2.11	0.65
2:V:108:VAL:HB	2:V:1403:LEU:CB	2.27	0.65
2:V:230:LEU:H	2:V:230:LEU:CD1	2.08	0.65
2:V:18:ASN:OD1	2:V:214:THR:HG21	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:97:GLU:OE2	2:V:101:TYR:OH	2.09	0.65
2:V:1039:HIS:CE1	2:V:1081:SER:HG	2.15	0.65
2:V:1296:LYS:CA	2:V:1301:SER:CB	2.72	0.65
2:V:1298:TRP:CE3	2:V:1299:TRP:CE2	2.85	0.65
2:V:511:ASN:O	2:V:512:LYS:CB	2.44	0.64
2:V:879:TYR:CE1	2:V:950:ASP:OD1	2.49	0.64
2:V:1189:VAL:CG2	2:V:1194:HIS:ND1	2.60	0.64
2:V:1256:TYR:O	2:V:1257:ASN:HB2	1.97	0.64
1:A:97:TRP:HA	1:A:371:ARG:HD2	1.78	0.64
2:V:641:SER:OG	2:V:644:MET:N	2.29	0.64
2:V:1298:TRP:CZ3	2:V:1299:TRP:CH2	2.72	0.64
2:V:206:THR:HG22	2:V:211:ALA:HB2	1.79	0.64
2:V:230:LEU:N	2:V:230:LEU:CD1	2.60	0.64
2:V:399:LYS:HA	2:V:499:CYS:O	1.98	0.64
2:V:911:ILE:CD1	2:V:917:TYR:HB2	2.28	0.64
2:V:959:ILE:O	2:V:960:LEU:HD23	1.98	0.64
2:V:94:LYS:HD2	2:V:105:THR:HG21	1.78	0.64
2:V:163:LEU:CD2	2:V:163:LEU:C	2.71	0.64
2:V:562:LEU:CD1	2:V:650:LEU:HD23	2.28	0.64
2:V:150:ASN:N	2:V:154:ASP:OD1	2.31	0.64
2:V:549:ASP:C	2:V:549:ASP:OD1	2.41	0.64
2:V:553:PHE:O	2:V:556:SER:HB3	1.97	0.64
2:V:1202:VAL:HG12	2:V:1203:THR:N	2.12	0.64
2:V:128:THR:HG22	2:V:129:ALA:H	1.63	0.64
2:V:368:VAL:HG11	2:V:391:ILE:HG13	1.80	0.64
2:V:979:PHE:HE2	2:V:1036:VAL:HG21	1.63	0.64
1:A:228:LYS:CB	1:A:318:LYS:O	2.47	0.63
2:V:248:THR:HG22	2:V:422:GLY:HA2	1.80	0.63
2:V:300:LYS:NZ	9:V:2046:HOH:O	2.30	0.63
1:A:99:PHE:HZ	1:A:287:PRO:HA	1.63	0.63
2:V:376:ASN:OD1	3:B:1:NAG:H82	1.98	0.63
2:V:935:LYS:N	2:V:1062:GLU:OE2	2.21	0.63
2:V:480:SER:OG	2:V:487:ASP:HB3	1.98	0.63
2:V:1057:GLN:CA	2:V:1057:GLN:NE2	2.49	0.63
2:V:1126:GLY:O	2:V:1128:ILE:C	2.41	0.63
2:V:1368:SER:HA	9:V:2100:HOH:O	1.98	0.63
1:A:411:GLN:HA	1:A:411:GLN:OE1	1.98	0.63
2:V:150:ASN:CB	2:V:154:ASP:OD1	2.45	0.63
2:V:258:THR:HG21	2:V:620:SER:HB3	1.79	0.63
2:V:864:ASP:N	2:V:923:VAL:O	2.26	0.63
2:V:1119:LEU:H	2:V:1119:LEU:CD1	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1278:GLY:HA3	2:V:1283:ALA:HB3	1.79	0.63
2:V:1374:LEU:HA	2:V:1381:GLU:CA	2.28	0.63
1:A:344:ASN:O	1:A:397:LYS:CB	2.46	0.63
2:V:17:TYR:CE2	2:V:206:THR:HG21	2.34	0.63
2:V:252:ASN:O	2:V:254:TYR:HD1	1.81	0.63
2:V:800:ILE:CG2	2:V:801:ALA:N	2.61	0.63
2:V:1015:PHE:O	2:V:1017:ALA:N	2.32	0.63
2:V:1030:MET:O	2:V:1112:VAL:HA	1.99	0.63
2:V:19:PRO:O	2:V:20:GLN:C	2.42	0.63
2:V:131:ILE:HD12	2:V:131:ILE:O	1.97	0.63
2:V:246:GLY:O	2:V:247:GLN:NE2	2.32	0.63
2:V:467:THR:O	2:V:500:LYS:NZ	2.31	0.63
2:V:475:THR:O	2:V:476:LYS:CG	2.47	0.63
2:V:1038:TRP:CD1	2:V:1084:MET:HG2	2.34	0.63
1:A:99:PHE:CE2	1:A:288:THR:HG23	2.33	0.62
2:V:337:ALA:CA	2:V:362:LYS:CD	2.61	0.62
2:V:641:SER:C	2:V:643:GLU:N	2.57	0.62
2:V:475:THR:C	2:V:476:LYS:HG3	2.23	0.62
1:A:89:CYS:O	1:A:93:ASN:HA	1.99	0.62
2:V:504:LEU:O	2:V:505:SER:CB	2.47	0.62
2:V:1094:LEU:HG	2:V:1108:ALA:O	1.98	0.62
2:V:196:ASN:O	2:V:197:TRP:C	2.43	0.62
2:V:808:ASP:HB2	2:V:824:THR:C	2.24	0.62
2:V:187:MET:HE1	2:V:233:MET:HB3	1.81	0.62
2:V:636:LEU:C	2:V:636:LEU:HD23	2.25	0.62
2:V:863:VAL:HA	2:V:923:VAL:CG1	2.29	0.62
1:A:174:MET:O	1:A:175:ASP:C	2.42	0.62
2:V:917:TYR:CD2	2:V:918:THR:N	2.67	0.62
2:V:131:ILE:C	2:V:131:ILE:CD1	2.73	0.62
2:V:155:PHE:CD1	2:V:155:PHE:C	2.78	0.62
2:V:407:VAL:HG23	2:V:407:VAL:O	1.99	0.62
2:V:591:VAL:HG11	2:V:595:VAL:HG23	1.81	0.62
2:V:479:HIS:CD2	2:V:488:ILE:HD11	2.35	0.61
2:V:285:VAL:HB	2:V:288:HIS:CD2	2.36	0.61
2:V:417:SER:HG	2:V:481:ALA:H	1.48	0.61
2:V:594:ILE:O	2:V:594:ILE:HG23	1.99	0.61
2:V:1088:LYS:NZ	9:V:2016:HOH:O	2.31	0.61
2:V:635:LEU:HB2	2:V:897:TYR:CD2	2.35	0.61
2:V:16:ASP:CB	9:V:2005:HOH:O	2.48	0.61
2:V:826:PHE:CZ	2:V:1015:PHE:HZ	2.18	0.61
2:V:1384:PHE:HD1	2:V:1384:PHE:H	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1183:ILE:HG22	2:V:1184:GLN:N	2.16	0.61
2:V:1423:GLU:OE1	2:V:1423:GLU:HA	1.99	0.61
2:V:19:PRO:HD3	9:V:2004:HOH:O	2.01	0.61
2:V:490:SER:HG	2:V:530:TRP:CD1	2.18	0.61
2:V:640:GLY:CA	2:V:644:MET:HE2	2.29	0.61
2:V:966:MET:O	2:V:967:ILE:HG13	2.01	0.61
2:V:1203:THR:HG21	2:V:1251:HIS:CE1	2.35	0.61
2:V:12:LEU:N	2:V:12:LEU:HD12	2.15	0.61
2:V:32:LEU:HD12	2:V:33:THR:N	2.16	0.61
2:V:97:GLU:HG2	2:V:99:SER:OG	2.00	0.61
2:V:911:ILE:HD11	2:V:917:TYR:CB	2.31	0.61
2:V:1256:TYR:O	2:V:1257:ASN:CB	2.48	0.61
2:V:1348:THR:HG22	2:V:1353:SER:CB	2.31	0.61
1:A:120:ASP:OD1	1:A:122:HIS:N	2.29	0.61
2:V:135:LYS:HD3	2:V:1066:ASP:OD1	2.01	0.61
2:V:631:LEU:HD23	2:V:631:LEU:N	2.15	0.61
2:V:1021:ILE:HD12	2:V:1025:LEU:HD12	1.82	0.61
2:V:1040:LEU:HD13	2:V:1052:VAL:HG11	1.81	0.61
2:V:1222:GLN:HG2	2:V:1223:MET:H	1.66	0.61
2:V:575:PHE:CD2	2:V:628:MET:CE	2.84	0.61
2:V:1032:LYS:O	2:V:1033:ASP:CB	2.46	0.61
2:V:1126:GLY:O	2:V:1128:ILE:CA	2.49	0.60
2:V:1156:ASN:ND2	2:V:1156:ASN:N	2.42	0.60
2:V:1179:VAL:O	2:V:1267:GLY:HA3	2.01	0.60
2:V:1315:THR:O	2:V:1315:THR:CG2	2.44	0.60
1:A:402:ILE:H	1:A:403:PRO:HD2	1.65	0.60
2:V:106:SER:OG	2:V:109:GLU:OE1	2.18	0.60
2:V:223:TYR:H	2:V:273:VAL:HG23	1.66	0.60
2:V:424:SER:HB2	2:V:461:LEU:HD12	1.83	0.60
2:V:432:ALA:HA	2:V:481:ALA:HB1	1.80	0.60
2:V:800:ILE:HG22	2:V:801:ALA:H	1.63	0.60
2:V:828:LYS:HG2	2:V:953:SER:O	2.00	0.60
2:V:1040:LEU:O	2:V:1079:PHE:HA	2.00	0.60
2:V:1309:LEU:HD11	2:V:1343:ILE:HB	1.82	0.60
2:V:517:GLN:OE1	2:V:573:LEU:HD21	2.01	0.60
2:V:1092:TRP:HB2	2:V:1110:PHE:CZ	2.36	0.60
2:V:1311:LEU:HD23	2:V:1311:LEU:C	2.27	0.60
1:A:176:CYS:CB	1:A:322:VAL:HG23	2.20	0.60
2:V:192:ASP:OD1	2:V:194:SER:OG	2.19	0.60
2:V:448:VAL:CG1	2:V:452:GLN:HB3	2.32	0.60
2:V:503:ALA:HA	2:V:511:ASN:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:595:VAL:HG12	2:V:595:VAL:O	2.00	0.60
2:V:680:ILE:N	2:V:681:PRO:HD3	2.13	0.60
2:V:989:GLU:OE1	2:V:1011:SER:CA	2.49	0.60
2:V:1312:GLU:O	2:V:1312:GLU:HG3	2.01	0.60
2:V:1340:THR:O	2:V:1398:PHE:HD1	1.83	0.60
2:V:1298:TRP:CZ3	2:V:1299:TRP:CZ2	2.90	0.60
2:V:1298:TRP:CE3	2:V:1299:TRP:CD2	2.90	0.60
2:V:1329:LEU:HB3	2:V:1409:ILE:CD1	2.31	0.60
2:V:1354:MET:HG2	2:V:1417:TYR:H	1.67	0.60
2:V:942:TYR:HE2	2:V:947:PRO:HB3	1.65	0.60
2:V:1278:GLY:O	2:V:1282:GLY:N	2.33	0.60
2:V:1329:LEU:CB	2:V:1409:ILE:HD11	2.31	0.60
2:V:657:TYR:CD1	2:V:657:TYR:N	2.70	0.60
2:V:860:ARG:HD2	2:V:967:ILE:CD1	2.31	0.60
2:V:336:TYR:C	2:V:338:PRO:HD3	2.27	0.59
2:V:823:LYS:C	2:V:824:THR:HG23	2.27	0.59
2:V:145:TYR:O	2:V:146:TYR:HB3	2.02	0.59
2:V:800:ILE:CG2	2:V:801:ALA:H	2.15	0.59
2:V:1183:ILE:CG2	2:V:1184:GLN:N	2.64	0.59
1:A:410:ARG:HH11	1:A:410:ARG:CG	2.11	0.59
2:V:1036:VAL:O	2:V:1084:MET:HB2	2.01	0.59
1:A:329:ASP:HB2	1:A:332:THR:OG1	2.01	0.59
2:V:1051:VAL:CG1	2:V:1071:VAL:HG13	2.27	0.59
1:A:120:ASP:CG	1:A:123:SER:H	2.11	0.59
2:V:153:ARG:NH2	2:V:197:TRP:HA	2.18	0.59
2:V:271:MET:HG2	2:V:272:SER:N	2.16	0.59
2:V:505:SER:CB	2:V:509:VAL:H	2.16	0.59
2:V:562:LEU:HD23	2:V:562:LEU:C	2.27	0.59
2:V:629:ASP:OD2	2:V:926:ARG:CZ	2.50	0.59
2:V:1292:SER:O	2:V:1293:SER:HB3	2.02	0.59
2:V:1142:TRP:HZ3	2:V:1188:THR:HG21	1.66	0.59
2:V:38:VAL:HG12	2:V:158:GLY:HA3	1.84	0.59
2:V:135:LYS:HD3	2:V:1066:ASP:CG	2.28	0.59
2:V:1338:LYS:O	2:V:1426:GLY:HA3	2.03	0.59
2:V:1389:ASN:N	2:V:1389:ASN:HD22	2.00	0.59
1:A:133:GLY:O	1:A:374:HIS:CD2	2.54	0.59
2:V:10:ALA:O	2:V:11:GLN:HB3	2.02	0.59
2:V:252:ASN:ND2	2:V:252:ASN:C	2.61	0.59
2:V:550:ASP:O	2:V:551:PRO:C	2.46	0.59
2:V:893:GLU:OE2	2:V:897:TYR:HE1	1.86	0.59
2:V:1107:GLN:O	2:V:1107:GLN:CG	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:505:SER:C	2:V:508:GLY:CA	2.75	0.59
2:V:585:LEU:HD12	2:V:585:LEU:H	1.68	0.59
2:V:1152:THR:HG22	2:V:1153:GLY:H	1.65	0.59
2:V:509:VAL:HG12	2:V:510:GLN:N	2.17	0.59
2:V:575:PHE:HB2	2:V:628:MET:HE3	1.84	0.59
2:V:930:THR:O	2:V:931:ASP:CG	2.46	0.59
2:V:952:HIS:HD2	2:V:987:ASP:H	1.51	0.59
2:V:36:LYS:HD3	2:V:157:SER:O	2.03	0.58
2:V:155:PHE:O	2:V:157:SER:N	2.36	0.58
2:V:260:ASN:HB3	2:V:617:PHE:CD1	2.38	0.58
2:V:396:ILE:C	2:V:397:LYS:HG3	2.26	0.58
2:V:562:LEU:C	2:V:562:LEU:CD2	2.76	0.58
2:V:863:VAL:HG12	2:V:864:ASP:OD1	2.03	0.58
2:V:484:MET:HG3	2:V:485:THR:N	2.19	0.58
2:V:808:ASP:HB3	2:V:825:THR:CA	2.33	0.58
2:V:1384:PHE:CD1	2:V:1384:PHE:N	2.71	0.58
2:V:95:TRP:CA	2:V:112:ASP:OD2	2.51	0.58
2:V:1185:THR:HG21	2:V:1261:PHE:CE1	2.36	0.58
2:V:615:ASN:HD22	2:V:1076:PRO:HD2	1.67	0.58
2:V:970:TYR:O	2:V:972:ARG:N	2.36	0.58
2:V:1258:ARG:HH11	2:V:1258:ARG:CG	1.92	0.58
2:V:1298:TRP:CZ3	2:V:1299:TRP:CE2	2.91	0.58
2:V:877:ARG:CG	2:V:877:ARG:NH1	2.55	0.58
2:V:168:GLU:OE2	9:V:2033:HOH:O	2.17	0.58
2:V:355:ASN:OD1	2:V:355:ASN:N	2.31	0.58
2:V:1022:PRO:O	2:V:1023:TYR:CB	2.52	0.58
2:V:496:LEU:HD23	2:V:497:LEU:N	2.18	0.58
2:V:254:TYR:CD2	2:V:607:LYS:HE3	2.39	0.58
2:V:255:LYS:CG	2:V:465:GLU:O	2.51	0.58
2:V:548:LYS:O	2:V:549:ASP:CB	2.51	0.58
2:V:597:VAL:HG22	2:V:614:LEU:O	2.04	0.58
2:V:1122:GLY:O	2:V:1123:LEU:HD12	2.04	0.58
2:V:1205:SER:CB	2:V:1211:TRP:CG	2.87	0.58
2:V:150:ASN:O	2:V:150:ASN:ND2	2.32	0.57
2:V:150:ASN:CA	2:V:154:ASP:OD1	2.52	0.57
2:V:372:TYR:CD2	2:V:377:PHE:CD1	2.91	0.57
2:V:419:TYR:O	2:V:478:TYR:HA	2.03	0.57
1:A:335:VAL:HA	2:V:512:LYS:CE	2.34	0.57
2:V:252:ASN:C	2:V:252:ASN:HD22	2.07	0.57
2:V:618:PRO:O	2:V:619:MET:HB2	2.03	0.57
1:A:344:ASN:ND2	1:A:401:PHE:CZ	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:4:ARG:HE	2:V:65:GLY:HA2	1.70	0.57
2:V:107:ASP:O	2:V:111:LEU:HG	2.04	0.57
2:V:124:VAL:HG23	2:V:124:VAL:O	2.03	0.57
2:V:325:TYR:HB2	2:V:406:ILE:HD13	1.87	0.57
2:V:433:ILE:HD12	2:V:482:VAL:HA	1.85	0.57
2:V:913:PRO:C	2:V:915:GLY:H	2.11	0.57
2:V:585:LEU:HD12	2:V:585:LEU:N	2.19	0.57
2:V:551:PRO:O	2:V:552:LYS:C	2.47	0.57
2:V:73:ILE:HB	2:V:123:TYR:HB2	1.85	0.57
2:V:521:PHE:CZ	2:V:597:VAL:HG11	2.40	0.57
2:V:594:ILE:O	2:V:594:ILE:CG2	2.52	0.57
2:V:42:TYR:CD1	2:V:49:GLU:HG2	2.40	0.57
2:V:86:HIS:NE2	2:V:1055:HIS:HE1	2.00	0.57
2:V:131:ILE:HG22	2:V:1058:THR:HG21	1.87	0.57
2:V:800:ILE:N	2:V:800:ILE:CD1	2.68	0.57
2:V:1328:TRP:O	2:V:1328:TRP:CE3	2.57	0.57
1:A:118:GLY:N	1:A:124:CYS:H	2.02	0.57
2:V:449:GLU:HB3	2:V:450:PRO:CD	2.27	0.57
2:V:600:SER:C	2:V:602:HIS:N	2.55	0.57
2:V:808:ASP:CB	2:V:825:THR:OG1	2.52	0.57
2:V:1056:GLY:C	2:V:1057:GLN:NE2	2.62	0.57
2:V:1156:ASN:HD21	2:V:1188:THR:CB	2.18	0.57
2:V:173:ALA:C	2:V:175:GLY:N	2.63	0.57
2:V:256:VAL:HG23	2:V:257:SER:N	2.19	0.57
2:V:522:ALA:O	2:V:561:THR:OG1	2.12	0.57
2:V:1096:THR:O	2:V:1102:GLN:HG3	2.05	0.57
2:V:1205:SER:CA	2:V:1211:TRP:HB3	2.28	0.57
1:A:334:MET:SD	2:V:512:LYS:O	2.63	0.56
2:V:525:ASP:HA	2:V:558:VAL:HA	1.87	0.56
2:V:924:PRO:HD2	2:V:927:SER:OG	2.04	0.56
2:V:968:ASP:O	2:V:969:LYS:C	2.49	0.56
1:A:111:CYS:SG	1:A:117:LEU:HA	2.44	0.56
2:V:525:ASP:CG	2:V:558:VAL:HG12	2.29	0.56
2:V:1151:ASN:C	2:V:1151:ASN:ND2	2.57	0.56
2:V:1304:PRO:N	2:V:1318:TRP:HD1	2.03	0.56
2:V:41:GLU:OE2	2:V:50:LYS:CD	2.53	0.56
2:V:220:ALA:O	2:V:299:ILE:HA	2.05	0.56
2:V:511:ASN:O	2:V:512:LYS:HB2	2.05	0.56
2:V:598:HIS:HD2	2:V:599:LEU:H	1.54	0.56
2:V:1335:HIS:CE1	2:V:1337:THR:CG2	2.88	0.56
2:V:122:LYS:NZ	9:V:2029:HOH:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:526:GLU:C	2:V:528:LYS:H	2.12	0.56
1:A:88:SER:C	1:A:91:VAL:H	2.12	0.56
2:V:930:THR:O	2:V:931:ASP:OD2	2.23	0.56
2:V:942:TYR:HB3	2:V:956:ILE:HD12	1.88	0.56
2:V:947:PRO:O	2:V:951:ILE:HG13	2.05	0.56
2:V:1092:TRP:HB2	2:V:1110:PHE:CE1	2.40	0.56
2:V:631:LEU:HA	2:V:654:ASP:O	2.06	0.56
2:V:848:TYR:C	2:V:850:LYS:H	2.13	0.56
2:V:1178:VAL:HG23	2:V:1180:ILE:CD1	2.36	0.56
2:V:1189:VAL:CG1	2:V:1194:HIS:ND1	2.68	0.56
2:V:1205:SER:CB	2:V:1211:TRP:HE3	2.18	0.56
2:V:66:GLU:O	2:V:127:ILE:HG21	2.06	0.56
2:V:391:ILE:HG12	2:V:391:ILE:O	2.04	0.56
2:V:656:ASN:C	2:V:657:TYR:CD1	2.84	0.56
2:V:894:GLY:C	2:V:895:ARG:HG3	2.31	0.56
2:V:1277:LEU:HD12	2:V:1424:LEU:HB3	1.85	0.56
2:V:1286:ASN:HB2	2:V:1305:PHE:CB	2.36	0.56
2:V:1363:TYR:HD1	2:V:1364:THR:O	1.89	0.56
2:V:1143:GLU:O	2:V:1158:TRP:HB2	2.06	0.56
2:V:1345:GLN:CA	2:V:1387:ASN:HD21	2.17	0.56
2:V:1359:PHE:CZ	2:V:1384:PHE:HB2	2.41	0.56
2:V:330:GLU:OE2	2:V:372:TYR:OH	2.24	0.56
2:V:1017:ALA:CB	2:V:1022:PRO:N	2.69	0.56
2:V:1106:MET:O	2:V:1107:GLN:HB3	2.06	0.56
2:V:17:TYR:CE2	2:V:204:GLN:HB2	2.42	0.55
2:V:173:ALA:O	2:V:175:GLY:N	2.39	0.55
2:V:942:TYR:CG	2:V:951:ILE:HD11	2.42	0.55
2:V:946:ASN:O	2:V:950:ASP:HB2	2.05	0.55
2:V:1138:HIS:HB3	2:V:1158:TRP:CD1	2.41	0.55
1:A:341:ILE:HG13	1:A:341:ILE:O	2.06	0.55
2:V:348:TYR:O	2:V:350:ALA:N	2.39	0.55
2:V:993:TYR:N	2:V:993:TYR:CD1	2.74	0.55
2:V:1279:MET:O	2:V:1308:ARG:CD	2.53	0.55
2:V:448:VAL:HG13	2:V:452:GLN:HB3	1.87	0.55
2:V:1275:VAL:HG13	2:V:1276:PRO:HD2	1.88	0.55
2:V:234:SER:OG	2:V:235:SER:N	2.33	0.55
2:V:150:ASN:HD22	2:V:153:ARG:H	1.55	0.55
2:V:385:TRP:O	2:V:386:PRO:C	2.49	0.55
2:V:605:LEU:HD13	2:V:610:HIS:CE1	2.42	0.55
2:V:606:SER:OG	2:V:611:GLN:CD	2.48	0.55
2:V:1173:ASP:CG	2:V:1247:TYR:CE1	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:357:SER:O	2:V:358:ASN:HB3	2.05	0.55
2:V:598:HIS:HD2	2:V:599:LEU:N	2.05	0.55
2:V:1184:GLN:HG2	2:V:1236:GLU:HG3	1.89	0.55
2:V:1258:ARG:NH1	2:V:1258:ARG:CG	2.57	0.55
2:V:977:ARG:NH2	2:V:1240:ASP:O	2.40	0.55
2:V:196:ASN:HA	9:V:2031:HOH:O	2.05	0.55
2:V:207:ILE:O	2:V:215:LEU:HD13	2.06	0.55
2:V:636:LEU:HD23	2:V:637:SER:N	2.22	0.55
2:V:941:TYR:CZ	2:V:957:GLY:HA3	2.42	0.55
2:V:1059:PHE:CE1	2:V:1069:LEU:CD1	2.90	0.55
2:V:1156:ASN:CG	2:V:1188:THR:HG1	2.13	0.55
2:V:1179:VAL:C	2:V:1180:ILE:HD12	2.32	0.55
2:V:511:ASN:O	2:V:512:LYS:CG	2.55	0.55
2:V:1289:ILE:HD12	2:V:1308:ARG:HH12	1.72	0.55
2:V:630:ASN:O	2:V:654:ASP:CG	2.49	0.55
4:C:3:BMA:H2	4:C:4:MAN:H5	1.89	0.55
1:A:183:TRP:O	1:A:184:GLN:C	2.49	0.54
2:V:172:ASN:ND2	2:V:172:ASN:H	2.05	0.54
2:V:331:GLU:HG3	2:V:412:ALA:CA	2.33	0.54
2:V:650:LEU:C	2:V:650:LEU:HD12	2.31	0.54
2:V:863:VAL:O	2:V:864:ASP:HB2	2.06	0.54
2:V:1279:MET:HB2	2:V:1423:GLU:OE1	2.07	0.54
2:V:1291:ALA:HB2	2:V:1304:PRO:HB2	1.83	0.54
2:V:64:ARG:CG	2:V:64:ARG:NH1	2.48	0.54
2:V:218:VAL:HG12	2:V:219:GLN:N	2.23	0.54
2:V:496:LEU:C	2:V:496:LEU:CD2	2.79	0.54
1:A:322:VAL:CG1	1:A:323:LEU:N	2.69	0.54
2:V:1211:TRP:CH2	2:V:1249:ARG:NE	2.75	0.54
2:V:1304:PRO:CB	2:V:1318:TRP:CD1	2.90	0.54
1:A:373:THR:HG22	1:A:374:HIS:N	2.23	0.54
2:V:285:VAL:HG12	2:V:286:ALA:N	2.23	0.54
2:V:364:TYR:CE2	2:V:526:GLU:HG3	2.41	0.54
2:V:511:ASN:C	2:V:512:LYS:HG2	2.32	0.54
2:V:989:GLU:CD	2:V:1011:SER:N	2.59	0.54
2:V:1152:THR:CG2	2:V:1153:GLY:N	2.70	0.54
2:V:1308:ARG:O	2:V:1421:ARG:CG	2.55	0.54
3:B:1:NAG:H82	3:B:1:NAG:C1	2.38	0.54
1:A:88:SER:O	1:A:89:CYS:C	2.51	0.54
2:V:207:ILE:O	2:V:215:LEU:CD1	2.55	0.54
2:V:424:SER:CB	2:V:461:LEU:HD12	2.38	0.54
2:V:888:TYR:HD2	2:V:893:GLU:HA	1.69	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:924:PRO:HG2	2:V:926:ARG:NH1	2.22	0.54
2:V:1156:ASN:HD21	2:V:1188:THR:CG2	2.18	0.54
2:V:1176:ARG:HH21	2:V:1178:VAL:HG12	1.73	0.54
2:V:158:GLY:O	2:V:160:ILE:HG22	2.07	0.54
2:V:801:ALA:HB1	2:V:874:LEU:HD13	1.90	0.54
2:V:16:ASP:CB	2:V:33:THR:HG22	2.37	0.54
2:V:385:TRP:O	2:V:386:PRO:O	2.26	0.54
2:V:837:ASP:O	2:V:839:PHE:HD1	1.90	0.54
2:V:873:ASN:O	2:V:874:LEU:CD1	2.38	0.54
2:V:979:PHE:CE2	2:V:1036:VAL:HG21	2.42	0.54
2:V:1374:LEU:O	2:V:1374:LEU:HD12	2.08	0.54
1:A:402:ILE:N	1:A:403:PRO:CD	2.70	0.54
2:V:248:THR:C	2:V:249:LEU:HD12	2.32	0.54
2:V:334:TRP:HB3	2:V:366:LYS:HG3	1.90	0.54
2:V:575:PHE:CB	2:V:628:MET:HE3	2.37	0.54
2:V:834:TYR:HE1	2:V:842:PRO:HD3	1.72	0.54
2:V:1309:LEU:HA	2:V:1421:ARG:HB3	1.90	0.54
2:V:1333:LEU:O	2:V:1335:HIS:N	2.40	0.54
1:A:99:PHE:CD2	1:A:288:THR:HG23	2.43	0.54
2:V:36:LYS:HB3	2:V:157:SER:O	2.08	0.54
2:V:246:GLY:O	2:V:247:GLN:CD	2.50	0.54
2:V:389:ARG:O	2:V:392:LEU:HB2	2.08	0.54
1:A:262:TYR:O	1:A:265:ASP:HB2	2.08	0.54
2:V:100:SER:HB2	2:V:113:ASP:HB3	1.90	0.54
2:V:365:LYS:HE3	2:V:531:TYR:CD1	2.42	0.54
2:V:831:PHE:CE1	2:V:955:LEU:HG	2.43	0.54
2:V:1310:ASN:OD1	2:V:1393:HIS:CE1	2.61	0.54
2:V:536:ILE:O	2:V:540:CYS:HB2	2.08	0.53
2:V:966:MET:O	2:V:967:ILE:CG1	2.56	0.53
1:A:118:GLY:HA2	1:A:123:SER:HB2	1.87	0.53
2:V:326:PHE:CD1	2:V:407:VAL:CG2	2.90	0.53
2:V:577:GLN:NE2	2:V:654:ASP:OD1	2.42	0.53
2:V:1185:THR:HG21	2:V:1261:PHE:HE1	1.59	0.53
2:V:875:ALA:O	2:V:913:PRO:HG3	2.08	0.53
2:V:1163:LYS:C	2:V:1165:HIS:H	2.16	0.53
2:V:1286:ASN:CB	2:V:1305:PHE:CB	2.83	0.53
2:V:526:GLU:C	2:V:528:LYS:N	2.66	0.53
2:V:548:LYS:O	2:V:549:ASP:HB3	2.09	0.53
2:V:809:TYR:OH	2:V:828:LYS:CE	2.56	0.53
2:V:1095:GLU:OE2	2:V:1102:GLN:HG2	2.09	0.53
2:V:4:ARG:NE	2:V:65:GLY:HA2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1345:GLN:HG2	2:V:1346:GLY:H	1.74	0.53
1:A:175:ASP:CA	1:A:320:LEU:O	2.52	0.53
2:V:343:SER:O	2:V:344:VAL:O	2.25	0.53
1:A:189:ASP:N	1:A:193:GLY:O	2.31	0.53
2:V:203:LEU:HD12	2:V:204:GLN:N	2.23	0.53
2:V:871:PHE:CG	2:V:881:LEU:CD1	2.88	0.53
2:V:1051:VAL:HG12	2:V:1071:VAL:CG1	2.33	0.53
2:V:1138:HIS:HB3	2:V:1158:TRP:NE1	2.24	0.53
5:E:2:NAG:O7	5:E:2:NAG:C3	2.56	0.53
2:V:356:PHE:O	2:V:357:SER:CB	2.56	0.53
2:V:486:ARG:NH2	9:V:2062:HOH:O	2.38	0.53
2:V:581:VAL:CG1	2:V:628:MET:HE2	2.39	0.53
2:V:1043:MET:HE1	2:V:1079:PHE:HE2	1.72	0.53
2:V:1201:PHE:HB3	2:V:1223:MET:O	2.09	0.53
2:V:353:LEU:O	2:V:354:ASP:C	2.52	0.53
2:V:1249:ARG:C	2:V:1250:LEU:HD12	2.34	0.53
2:V:94:LYS:HG2	2:V:97:GLU:OE1	2.09	0.53
2:V:831:PHE:CE1	2:V:955:LEU:HD12	2.44	0.53
2:V:1121:MET:CG	2:V:1121:MET:O	2.56	0.53
2:V:1295:LYS:HB3	2:V:1321:GLU:HA	1.91	0.53
2:V:1409:ILE:O	2:V:1409:ILE:CD1	2.49	0.53
2:V:91:VAL:HG12	2:V:131:ILE:HG12	1.91	0.52
2:V:138:PRO:HB2	2:V:139:PRO:HD2	1.91	0.52
2:V:527:ASN:ND2	2:V:527:ASN:N	2.46	0.52
2:V:554:TYR:CE1	2:V:558:VAL:CG1	2.93	0.52
2:V:942:TYR:CE2	2:V:947:PRO:HB3	2.42	0.52
2:V:1304:PRO:HB3	2:V:1318:TRP:CD1	2.45	0.52
2:V:367:ALA:O	2:V:492:LEU:CD1	2.58	0.52
2:V:681:PRO:O	2:V:682:SER:CB	2.58	0.52
1:A:107:ILE:O	1:A:107:ILE:CG1	2.57	0.52
2:V:157:SER:HA	2:V:196:ASN:ND2	2.24	0.52
2:V:483:ASP:O	2:V:485:THR:N	2.42	0.52
2:V:554:TYR:O	2:V:558:VAL:HG13	2.09	0.52
2:V:593:GLU:HB3	2:V:1046:PRO:CB	2.40	0.52
2:V:1040:LEU:CD1	2:V:1052:VAL:HG11	2.40	0.52
2:V:1277:LEU:HD12	2:V:1424:LEU:CB	2.39	0.52
2:V:993:TYR:HD1	2:V:993:TYR:H	1.57	0.52
2:V:1101:ASN:N	2:V:1101:ASN:ND2	2.58	0.52
1:A:347:CYS:HB2	1:A:393:GLY:O	2.10	0.52
1:A:362:SER:HA	1:A:380:VAL:CB	2.39	0.52
2:V:474:ILE:HG22	2:V:498:VAL:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1308:ARG:O	2:V:1421:ARG:HG2	2.10	0.52
1:A:408:ILE:CD1	2:V:674:ILE:HG23	2.40	0.52
2:V:291:ALA:O	4:C:1:NAG:C6	2.51	0.52
2:V:596:PRO:O	2:V:597:VAL:HG13	2.09	0.52
2:V:943:SER:HB2	2:V:950:ASP:HB3	1.90	0.52
2:V:1289:ILE:HG21	2:V:1305:PHE:HA	1.91	0.52
2:V:1336:LEU:HD21	2:V:1403:LEU:O	2.10	0.52
2:V:1365:ASP:O	2:V:1366:ASP:C	2.53	0.52
2:V:65:GLY:O	2:V:66:GLU:O	2.28	0.52
2:V:136:ALA:HB3	2:V:1067:ASN:ND2	2.25	0.52
2:V:808:ASP:HB3	2:V:825:THR:CB	2.39	0.52
2:V:1184:GLN:HE21	2:V:1236:GLU:HG3	1.75	0.52
2:V:1289:ILE:HG22	2:V:1304:PRO:O	2.08	0.52
2:V:1308:ARG:O	2:V:1421:ARG:HB3	2.09	0.52
2:V:1151:ASN:O	2:V:1262:ARG:NH1	2.43	0.51
2:V:241:SER:HA	2:V:259:ILE:O	2.10	0.51
2:V:262:VAL:HG21	2:V:1073:PRO:HB3	1.92	0.51
2:V:1319:GLN:CB	2:V:1418:ILE:O	2.58	0.51
1:A:304:VAL:HG21	1:A:395:TYR:OH	2.10	0.51
2:V:478:TYR:CE1	2:V:494:GLY:C	2.89	0.51
2:V:1201:PHE:CB	2:V:1223:MET:O	2.58	0.51
2:V:17:TYR:CD2	2:V:204:GLN:HB3	2.45	0.51
2:V:640:GLY:HA3	2:V:644:MET:HE1	1.88	0.51
2:V:860:ARG:HD2	2:V:967:ILE:HD13	1.91	0.51
2:V:1017:ALA:CB	2:V:1022:PRO:CA	2.89	0.51
2:V:509:VAL:HG12	2:V:510:GLN:H	1.75	0.51
2:V:674:ILE:O	2:V:675:PHE:CB	2.53	0.51
2:V:422:GLY:HA3	2:V:476:LYS:CD	2.40	0.51
2:V:911:ILE:CG2	2:V:915:GLY:CA	2.85	0.51
2:V:1182:GLY:C	2:V:1183:ILE:HD12	2.36	0.51
2:V:1357:LYS:H	2:V:1414:TRP:HA	1.75	0.51
2:V:140:CYS:HB3	2:V:164:LEU:HG	1.93	0.51
2:V:1356:VAL:O	2:V:1386:GLY:HA3	2.11	0.51
2:V:172:ASN:ND2	2:V:172:ASN:N	2.59	0.51
2:V:804:GLU:OE1	2:V:993:TYR:HE2	1.93	0.51
2:V:112:ASP:OD1	2:V:113:ASP:N	2.44	0.51
2:V:1414:TRP:CG	2:V:1418:ILE:HG12	2.46	0.51
2:V:51:PRO:O	2:V:52:ARG:O	2.29	0.50
2:V:87:PRO:HG2	2:V:92:TYR:CD1	2.46	0.50
2:V:592:ASP:OD1	2:V:592:ASP:C	2.54	0.50
2:V:831:PHE:CE1	2:V:955:LEU:CD1	2.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:883:ALA:HB2	2:V:921:TRP:CH2	2.46	0.50
2:V:131:ILE:CD1	2:V:165:ILE:HG21	2.41	0.50
2:V:1030:MET:CE	2:V:1110:PHE:CD2	2.91	0.50
2:V:1041:LEU:HD12	2:V:1041:LEU:N	2.26	0.50
2:V:1214:PHE:CZ	2:V:1239:ILE:CG2	2.86	0.50
2:V:155:PHE:C	2:V:157:SER:N	2.68	0.50
2:V:1152:THR:CG2	2:V:1153:GLY:H	2.24	0.50
2:V:1299:TRP:CD1	2:V:1299:TRP:N	2.78	0.50
2:V:294:TYR:HE1	2:V:296:TYR:HE1	1.58	0.50
2:V:826:PHE:CE1	2:V:1015:PHE:CZ	2.99	0.50
1:A:182:PRO:HB2	1:A:282:VAL:N	2.26	0.50
2:V:1328:TRP:CE3	2:V:1328:TRP:C	2.89	0.50
1:A:210:ALA:HB3	1:A:248:PHE:CD1	2.47	0.50
2:V:221:CYS:HA	2:V:300:LYS:O	2.12	0.50
2:V:606:SER:O	2:V:609:LYS:N	2.27	0.50
2:V:1240:ASP:HB3	2:V:1241:PRO:HD3	1.94	0.50
2:V:1304:PRO:HA	2:V:1318:TRP:CG	2.41	0.50
2:V:1339:ILE:HD13	2:V:1407:ILE:HD13	1.84	0.50
2:V:1420:LEU:O	2:V:1420:LEU:HD12	2.11	0.50
1:A:89:CYS:SG	1:A:101:LYS:O	2.70	0.50
2:V:941:TYR:CE2	2:V:957:GLY:HA3	2.47	0.50
2:V:1123:LEU:HD22	2:V:1264:GLU:HA	1.92	0.50
2:V:108:VAL:CB	2:V:1403:LEU:CB	2.90	0.50
2:V:427:LYS:HA	2:V:430:GLU:HB2	1.94	0.50
2:V:839:PHE:O	2:V:840:GLN:CB	2.60	0.50
2:V:1420:LEU:HD12	2:V:1420:LEU:C	2.37	0.50
1:A:98:HIS:CD2	1:A:375:PHE:CZ	2.85	0.49
2:V:16:ASP:C	2:V:18:ASN:H	2.20	0.49
2:V:526:GLU:O	2:V:528:LYS:N	2.45	0.49
2:V:536:ILE:O	2:V:543:PRO:HG3	2.12	0.49
2:V:985:VAL:O	2:V:985:VAL:HG12	2.11	0.49
2:V:1031:TYR:OH	2:V:1181:THR:HG21	2.11	0.49
2:V:1179:VAL:HG22	2:V:1244:ILE:HG12	1.93	0.49
2:V:1345:GLN:CA	2:V:1387:ASN:ND2	2.74	0.49
2:V:285:VAL:CB	2:V:288:HIS:HD2	2.22	0.49
2:V:337:ALA:C	2:V:362:LYS:HD3	2.32	0.49
2:V:349:LYS:O	2:V:354:ASP:CB	2.60	0.49
2:V:576:HIS:CD2	2:V:657:TYR:CE2	3.01	0.49
2:V:803:GLU:OE2	2:V:834:TYR:CZ	2.65	0.49
2:V:1189:VAL:HG23	2:V:1231:GLY:O	2.12	0.49
2:V:343:SER:O	2:V:344:VAL:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:365:LYS:CE	2:V:531:TYR:CD1	2.96	0.49
2:V:391:ILE:HG22	2:V:564:GLY:HA3	1.93	0.49
2:V:1202:VAL:CG1	2:V:1203:THR:N	2.76	0.49
1:A:88:SER:O	1:A:91:VAL:CA	2.60	0.49
1:A:370:TYR:O	1:A:371:ARG:C	2.55	0.49
2:V:173:ALA:C	2:V:175:GLY:H	2.19	0.49
2:V:188:PHE:O	2:V:232:GLY:HA2	2.12	0.49
2:V:551:PRO:O	2:V:553:PHE:N	2.46	0.49
2:V:632:GLY:O	2:V:634:TRP:CD1	2.65	0.49
2:V:106:SER:C	2:V:108:VAL:H	2.20	0.49
2:V:172:ASN:H	2:V:172:ASN:HD22	1.59	0.49
2:V:325:TYR:HB2	2:V:406:ILE:CD1	2.42	0.49
2:V:359:PHE:CE1	2:V:553:PHE:HA	2.40	0.49
2:V:364:TYR:N	2:V:364:TYR:CD1	2.80	0.49
2:V:396:ILE:CG2	2:V:397:LYS:N	2.75	0.49
2:V:979:PHE:HE2	2:V:1036:VAL:CG2	2.23	0.49
2:V:478:TYR:CE1	2:V:494:GLY:O	2.65	0.49
2:V:1051:VAL:HA	2:V:1073:PRO:HA	1.95	0.49
2:V:1189:VAL:HG22	2:V:1194:HIS:CG	2.48	0.49
2:V:256:VAL:O	2:V:257:SER:CB	2.59	0.49
2:V:877:ARG:NE	2:V:992:TRP:CD2	2.81	0.49
2:V:911:ILE:HG23	2:V:915:GLY:HA3	1.92	0.49
2:V:1021:ILE:O	2:V:1021:ILE:HG22	2.12	0.49
2:V:1298:TRP:HE3	2:V:1299:TRP:CE2	2.30	0.49
1:A:370:TYR:O	1:A:373:THR:N	2.43	0.49
2:V:138:PRO:HB2	2:V:139:PRO:CD	2.42	0.49
2:V:160:ILE:CD1	2:V:187:MET:HE1	2.37	0.49
2:V:205:TYR:CE2	4:C:2:NAG:H5	2.46	0.49
2:V:248:THR:CG2	2:V:422:GLY:HA2	2.41	0.49
2:V:396:ILE:HG22	2:V:397:LYS:H	1.76	0.49
2:V:1211:TRP:CZ2	2:V:1249:ARG:NE	2.81	0.49
2:V:1246:ARG:NH1	2:V:1246:ARG:CG	2.42	0.49
1:A:174:MET:O	1:A:175:ASP:O	2.31	0.49
2:V:106:SER:C	2:V:108:VAL:N	2.70	0.49
2:V:355:ASN:HB3	2:V:361:GLY:HA3	1.93	0.49
2:V:871:PHE:CD1	2:V:881:LEU:CD1	2.96	0.49
2:V:1132:GLN:NE2	2:V:1175:GLN:OE1	2.34	0.49
2:V:1203:THR:CG2	2:V:1251:HIS:CE1	2.95	0.49
2:V:1423:GLU:OE1	2:V:1423:GLU:CA	2.61	0.49
2:V:635:LEU:HB2	2:V:897:TYR:CE2	2.47	0.49
2:V:1030:MET:CE	2:V:1110:PHE:HD2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1156:ASN:HD22	2:V:1156:ASN:N	1.86	0.49
2:V:155:PHE:O	2:V:156:ASN:C	2.55	0.48
2:V:342:SER:O	2:V:343:SER:C	2.55	0.48
2:V:400:VAL:O	2:V:401:ARG:CB	2.54	0.48
2:V:1363:TYR:CD1	2:V:1364:THR:O	2.65	0.48
2:V:81:GLN:HB3	2:V:82:PRO:HD2	1.95	0.48
2:V:146:TYR:CD1	2:V:146:TYR:C	2.91	0.48
2:V:187:MET:HA	2:V:231:ILE:O	2.13	0.48
2:V:1407:ILE:HD12	2:V:1424:LEU:HD13	1.94	0.48
1:A:400:LYS:NZ	2:V:657:TYR:OH	2.46	0.48
2:V:127:ILE:HG22	2:V:127:ILE:O	2.12	0.48
2:V:151:MET:O	2:V:155:PHE:HB3	2.13	0.48
2:V:156:ASN:HD22	2:V:195:LYS:CB	2.26	0.48
2:V:807:TRP:N	2:V:826:PHE:O	2.31	0.48
2:V:331:GLU:HG3	2:V:412:ALA:CB	2.42	0.48
2:V:529:SER:OG	2:V:530:TRP:N	2.46	0.48
1:A:248:PHE:HA	1:A:264:TYR:HB2	1.95	0.48
1:A:263:ASP:O	1:A:264:TYR:HB2	2.13	0.48
2:V:17:TYR:HB3	2:V:211:ALA:CB	2.38	0.48
2:V:128:THR:CG2	2:V:129:ALA:N	2.76	0.48
2:V:809:TYR:HB3	2:V:1022:PRO:CD	2.43	0.48
2:V:1291:ALA:C	2:V:1328:TRP:CZ3	2.91	0.48
2:V:511:ASN:C	2:V:512:LYS:CG	2.86	0.48
2:V:1374:LEU:CA	2:V:1381:GLU:HA	2.36	0.48
3:B:1:NAG:H3	3:B:1:NAG:H83	1.96	0.48
2:V:1123:LEU:HD23	2:V:1263:ILE:HG13	1.95	0.48
2:V:152:VAL:HG11	2:V:1103:GLU:OE2	2.13	0.48
2:V:368:VAL:HG11	2:V:391:ILE:CG1	2.42	0.48
2:V:941:TYR:HB3	2:V:959:ILE:HD11	1.96	0.48
2:V:1043:MET:CE	2:V:1079:PHE:HE2	2.27	0.48
2:V:1355:TYR:HD1	2:V:1389:ASN:O	1.91	0.48
1:A:106:ASP:O	1:A:107:ILE:HG22	2.09	0.48
2:V:979:PHE:CE2	2:V:1036:VAL:CG2	2.96	0.48
2:V:1409:ILE:O	2:V:1411:PRO:HD3	2.14	0.48
2:V:150:ASN:O	2:V:151:MET:C	2.55	0.48
2:V:445:GLY:CA	2:V:454:TYR:CE2	2.97	0.48
2:V:554:TYR:CD1	2:V:558:VAL:HG11	2.48	0.48
2:V:989:GLU:HG3	2:V:1013:HIS:ND1	2.28	0.48
2:V:1123:LEU:O	2:V:1148:ARG:HB3	2.13	0.48
1:A:409:MET:C	1:A:411:GLN:N	2.54	0.47
2:V:81:GLN:HA	2:V:81:GLN:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:826:PHE:CD1	2:V:826:PHE:N	2.82	0.47
2:V:893:GLU:OE2	2:V:897:TYR:CE1	2.67	0.47
1:A:398:LEU:HD23	1:A:398:LEU:C	2.38	0.47
2:V:1052:VAL:HG12	2:V:1072:LEU:O	2.14	0.47
2:V:1279:MET:SD	2:V:1331:ILE:HD13	2.54	0.47
2:V:1296:LYS:CB	2:V:1301:SER:CB	2.91	0.47
1:A:377:THR:O	1:A:398:LEU:HB3	2.15	0.47
2:V:7:HIS:HB2	2:V:42:TYR:O	2.14	0.47
2:V:499:CYS:O	2:V:500:LYS:O	2.33	0.47
2:V:678:ILE:O	2:V:679:PHE:HB2	2.13	0.47
2:V:809:TYR:N	2:V:809:TYR:CD1	2.82	0.47
2:V:854:ILE:O	2:V:855:LEU:C	2.57	0.47
2:V:1017:ALA:HB1	2:V:1022:PRO:CA	2.43	0.47
2:V:1025:LEU:O	2:V:1026:GLN:CB	2.60	0.47
2:V:1293:SER:O	2:V:1320:PRO:HA	2.14	0.47
2:V:49:GLU:HB3	2:V:50:LYS:H	1.50	0.47
2:V:926:ARG:C	2:V:926:ARG:CD	2.87	0.47
2:V:1119:LEU:O	2:V:1120:PRO:C	2.57	0.47
2:V:1222:GLN:HG2	2:V:1223:MET:N	2.29	0.47
2:V:1258:ARG:O	2:V:1260:THR:N	2.47	0.47
2:V:1345:GLN:CB	2:V:1421:ARG:HB2	2.43	0.47
2:V:1355:TYR:CD2	2:V:1387:ASN:O	2.67	0.47
2:V:249:LEU:HD12	2:V:249:LEU:N	2.29	0.47
2:V:917:TYR:CG	2:V:918:THR:N	2.83	0.47
2:V:942:TYR:HB3	2:V:956:ILE:CD1	2.43	0.47
2:V:1098:VAL:O	2:V:1102:GLN:HB2	2.13	0.47
1:A:118:GLY:HA3	1:A:123:SER:CB	2.41	0.47
2:V:839:PHE:CE2	2:V:872:LYS:HG2	2.50	0.47
1:A:106:ASP:C	1:A:107:ILE:CG2	2.81	0.47
2:V:324:GLU:HA	2:V:405:THR:O	2.15	0.47
2:V:395:VAL:HG22	2:V:495:PRO:HG2	1.95	0.47
2:V:419:TYR:N	2:V:479:HIS:O	2.47	0.47
2:V:1126:GLY:HA2	2:V:1148:ARG:HH21	1.79	0.47
2:V:1291:ALA:CB	2:V:1304:PRO:HG3	2.41	0.47
2:V:95:TRP:HA	2:V:112:ASP:OD2	2.15	0.47
2:V:173:ALA:O	2:V:174:ASN:C	2.58	0.47
2:V:426:SER:O	2:V:430:GLU:N	2.48	0.47
2:V:1289:ILE:HD12	2:V:1308:ARG:NH1	2.30	0.47
1:A:132:CYS:C	1:A:285:CYS:SG	2.98	0.47
2:V:1:ALA:O	2:V:2:GLN:HB2	2.15	0.47
2:V:349:LYS:HA	2:V:353:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:397:LYS:O	2:V:398:ALA:HB2	2.15	0.47
2:V:414:ARG:HB2	2:V:415:PRO:HD2	1.97	0.47
2:V:483:ASP:O	2:V:484:MET:C	2.58	0.47
2:V:598:HIS:CD2	2:V:599:LEU:N	2.82	0.47
2:V:823:LYS:O	2:V:824:THR:OG1	2.24	0.47
2:V:837:ASP:O	2:V:839:PHE:CD1	2.68	0.47
2:V:877:ARG:NH1	2:V:878:PRO:O	2.48	0.47
2:V:1048:ASP:HB2	2:V:1050:HIS:NE2	2.29	0.47
2:V:1348:THR:HG23	2:V:1390:SER:OG	2.14	0.47
2:V:90:ALA:HB1	2:V:1056:GLY:C	2.40	0.47
2:V:256:VAL:HG23	2:V:257:SER:H	1.80	0.47
2:V:1075:LEU:O	2:V:1078:THR:HB	2.15	0.47
2:V:1344:THR:O	2:V:1387:ASN:ND2	2.43	0.47
2:V:151:MET:CE	2:V:1103:GLU:HB3	2.45	0.46
2:V:368:VAL:CG2	2:V:385:TRP:HZ2	2.28	0.46
2:V:834:TYR:CE1	2:V:842:PRO:HD3	2.49	0.46
2:V:849:GLU:HA	2:V:852:LEU:HG	1.98	0.46
2:V:879:TYR:HE1	2:V:950:ASP:OD1	1.96	0.46
2:V:1201:PHE:CE2	2:V:1251:HIS:CD2	3.02	0.46
2:V:1395:LYS:NZ	9:V:2098:HOH:O	2.46	0.46
2:V:7:HIS:CB	2:V:42:TYR:O	2.63	0.46
2:V:337:ALA:HB3	2:V:362:LYS:HD3	0.48	0.46
2:V:946:ASN:HB3	2:V:992:TRP:HZ2	1.80	0.46
2:V:1048:ASP:HB2	2:V:1050:HIS:CE1	2.50	0.46
2:V:321:LYS:O	2:V:322:ASN:C	2.58	0.46
2:V:826:PHE:CE1	2:V:1015:PHE:HZ	2.33	0.46
2:V:982:PHE:CE2	2:V:984:MET:HB3	2.51	0.46
2:V:1335:HIS:O	2:V:1337:THR:HG23	2.16	0.46
2:V:222:ALA:O	2:V:223:TYR:CB	2.64	0.46
2:V:341:PRO:HG3	2:V:569:ARG:C	2.40	0.46
2:V:414:ARG:HD3	2:V:530:TRP:CG	2.50	0.46
2:V:484:MET:CG	2:V:485:THR:N	2.79	0.46
2:V:838:THR:O	2:V:839:PHE:HB2	2.16	0.46
2:V:1340:THR:C	2:V:1398:PHE:HD1	2.22	0.46
1:A:293:ASN:ND2	1:A:399:SER:OG	2.48	0.46
2:V:432:ALA:CA	2:V:481:ALA:CB	2.77	0.46
2:V:550:ASP:O	2:V:553:PHE:N	2.48	0.46
2:V:899:ASP:O	2:V:899:ASP:OD1	2.34	0.46
2:V:1189:VAL:CG1	2:V:1194:HIS:CE1	2.99	0.46
2:V:1204:TYR:O	2:V:1211:TRP:HB3	2.11	0.46
2:V:1279:MET:SD	2:V:1284:ILE:HD12	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:TRP:O	1:A:184:GLN:O	2.34	0.46
2:V:81:GLN:OE1	2:V:82:PRO:CD	2.64	0.46
2:V:283:SER:C	2:V:285:VAL:H	2.23	0.46
2:V:1156:ASN:ND2	2:V:1188:THR:CB	2.79	0.46
2:V:1174:LEU:CD1	2:V:1178:VAL:HG22	2.43	0.46
2:V:1309:LEU:O	2:V:1310:ASN:C	2.57	0.46
3:B:1:NAG:C1	3:B:1:NAG:C8	2.94	0.46
2:V:12:LEU:N	2:V:12:LEU:CD1	2.79	0.46
2:V:884:HIS:NE2	2:V:942:TYR:HE1	2.14	0.46
2:V:1028:LEU:N	2:V:1028:LEU:HD12	2.31	0.46
2:V:92:TYR:CD2	2:V:97:GLU:HA	2.51	0.46
2:V:341:PRO:O	2:V:344:VAL:HG22	2.16	0.46
2:V:554:TYR:HE1	2:V:558:VAL:HG11	1.78	0.46
2:V:924:PRO:HD2	2:V:927:SER:CB	2.45	0.46
2:V:1238:HIS:CD2	2:V:1239:ILE:N	2.84	0.46
2:V:1333:LEU:HD13	2:V:1337:THR:OG1	2.16	0.46
2:V:1345:GLN:OE1	2:V:1421:ARG:HD2	2.16	0.46
2:V:346:ARG:C	2:V:348:TYR:N	2.73	0.46
2:V:853:GLY:HA3	2:V:1019:ASN:HB3	1.98	0.46
2:V:958:PRO:HB3	2:V:980:VAL:HG11	1.97	0.46
2:V:1278:GLY:HA2	2:V:1281:SER:HG	1.77	0.46
1:A:264:TYR:HD1	1:A:401:PHE:HE2	1.63	0.46
2:V:152:VAL:HG23	2:V:235:SER:HB2	1.96	0.46
2:V:347:ARG:O	2:V:351:GLN:HG3	2.15	0.46
2:V:871:PHE:CD2	2:V:881:LEU:HD13	2.49	0.46
2:V:1223:MET:CG	2:V:1224:HIS:CD2	2.98	0.46
2:V:150:ASN:O	2:V:153:ARG:N	2.40	0.45
2:V:382:TYR:HE2	9:V:2055:HOH:O	1.98	0.45
2:V:526:GLU:O	2:V:529:SER:N	2.40	0.45
2:V:828:LYS:CG	2:V:953:SER:O	2.63	0.45
2:V:943:SER:CB	2:V:950:ASP:HB3	2.46	0.45
2:V:944:GLY:O	2:V:947:PRO:HD3	2.16	0.45
2:V:1253:THR:HG23	2:V:1254:LYS:N	2.31	0.45
2:V:7:HIS:HD2	2:V:46:PHE:CE1	2.34	0.45
2:V:242:VAL:HG22	2:V:243:HIS:N	2.31	0.45
2:V:280:LEU:HD11	2:V:294:TYR:CD1	2.51	0.45
2:V:366:LYS:HD2	2:V:491:GLY:HA3	1.98	0.45
2:V:795:LYS:O	2:V:796:ARG:CB	2.59	0.45
2:V:1023:TYR:CE2	2:V:1105:GLY:HA2	2.51	0.45
2:V:1211:TRP:N	2:V:1211:TRP:CD1	2.83	0.45
4:C:1:NAG:O6	4:C:1:NAG:C1	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:187:MET:O	2:V:187:MET:HG3	2.15	0.45
2:V:259:ILE:CG2	2:V:267:VAL:HG11	2.46	0.45
2:V:562:LEU:HD23	2:V:563:ASN:N	2.31	0.45
2:V:582:GLN:HE21	2:V:625:THR:CG2	2.29	0.45
2:V:642:CYS:HB3	2:V:1002:CYS:HB3	1.42	0.45
2:V:1232:THR:HG23	2:V:1233:THR:N	2.31	0.45
2:V:926:ARG:CD	2:V:926:ARG:O	2.65	0.45
1:A:242:ILE:HB	2:V:679:PHE:O	2.15	0.45
2:V:291:ALA:HB2	4:C:2:NAG:H62	1.99	0.45
2:V:872:LYS:O	2:V:872:LYS:HG3	2.17	0.45
2:V:917:TYR:CE2	2:V:918:THR:O	2.70	0.45
2:V:1017:ALA:HB1	2:V:1021:ILE:C	2.41	0.45
2:V:1032:LYS:HD2	2:V:1089:ILE:HG12	1.98	0.45
2:V:1062:GLU:C	2:V:1064:ARG:H	2.25	0.45
2:V:1121:MET:O	2:V:1121:MET:HG2	2.17	0.45
1:A:408:ILE:HD11	2:V:674:ILE:HG23	1.98	0.45
2:V:17:TYR:CD2	2:V:206:THR:CG2	2.97	0.45
2:V:17:TYR:CE2	2:V:204:GLN:HB3	2.49	0.45
2:V:140:CYS:HA	2:V:166:CYS:HA	1.98	0.45
2:V:147:SER:HB3	2:V:154:ASP:HB3	1.99	0.45
2:V:604:PHE:CD1	2:V:626:VAL:CG1	3.00	0.45
2:V:809:TYR:OH	2:V:828:LYS:HE3	2.16	0.45
2:V:1028:LEU:HB3	2:V:1110:PHE:HB2	1.99	0.45
2:V:1044:GLY:HA3	2:V:1048:ASP:OD1	2.14	0.45
2:V:228:TRP:HB3	2:V:230:LEU:CD1	2.43	0.45
2:V:279:TRP:O	2:V:296:TYR:HA	2.16	0.45
2:V:285:VAL:CG1	2:V:286:ALA:N	2.80	0.45
2:V:449:GLU:CB	2:V:450:PRO:HD2	2.25	0.45
2:V:1141:TYR:HB2	2:V:1155:TYR:CE2	2.52	0.45
2:V:1203:THR:CG2	2:V:1203:THR:O	2.59	0.45
2:V:1205:SER:CB	2:V:1211:TRP:CD2	3.00	0.45
2:V:1309:LEU:HD12	2:V:1423:GLU:CA	2.32	0.45
2:V:1343:ILE:HG22	2:V:1344:THR:N	2.30	0.45
2:V:612:ASP:OD2	2:V:884:HIS:ND1	2.48	0.45
2:V:912:MET:O	2:V:913:PRO:C	2.60	0.45
2:V:1187:GLY:O	2:V:1231:GLY:C	2.59	0.45
2:V:1290:THR:HG22	2:V:1291:ALA:N	2.32	0.45
1:A:322:VAL:HG12	1:A:323:LEU:N	2.30	0.45
2:V:303:GLY:HA3	9:V:2049:HOH:O	2.15	0.45
2:V:851:HIS:O	2:V:1025:LEU:HD11	2.17	0.45
2:V:860:ARG:HD2	2:V:967:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1101:ASN:O	2:V:1102:GLN:C	2.59	0.45
2:V:9:ALA:HB1	2:V:76:LYS:O	2.17	0.45
2:V:283:SER:O	2:V:285:VAL:N	2.49	0.45
2:V:290:GLN:NE2	4:C:4:MAN:O6	2.50	0.45
2:V:575:PHE:CG	2:V:628:MET:HE3	2.52	0.45
2:V:798:TYR:HB3	2:V:800:ILE:HD11	1.98	0.45
2:V:799:TYR:CD2	2:V:836:ASP:HA	2.52	0.45
2:V:888:TYR:CE2	2:V:893:GLU:HA	2.51	0.45
2:V:932:ASN:O	2:V:933:THR:C	2.59	0.45
2:V:606:SER:O	2:V:608:GLY:N	2.50	0.44
2:V:632:GLY:N	2:V:654:ASP:O	2.49	0.44
2:V:1038:TRP:HB2	2:V:1082:ILE:HG12	1.99	0.44
2:V:1170:ILE:HG23	2:V:1170:ILE:O	2.18	0.44
2:V:157:SER:N	9:V:2031:HOH:O	2.50	0.44
2:V:417:SER:OG	2:V:481:ALA:N	2.41	0.44
2:V:944:GLY:O	2:V:945:VAL:C	2.60	0.44
2:V:1142:TRP:CD1	2:V:1142:TRP:H	2.34	0.44
2:V:1206:GLU:HA	2:V:1246:ARG:H	1.82	0.44
2:V:1291:ALA:CB	2:V:1304:PRO:CG	2.95	0.44
2:V:1349:SER:O	2:V:1350:MET:C	2.60	0.44
2:V:1356:VAL:CG1	2:V:1358:THR:O	2.65	0.44
2:V:61:PRO:HD2	2:V:145:TYR:OH	2.17	0.44
2:V:484:MET:O	2:V:488:ILE:HG13	2.17	0.44
2:V:858:ILE:HG12	2:V:958:PRO:HG2	1.99	0.44
2:V:1216:GLY:N	2:V:1222:GLN:HA	2.30	0.44
2:V:2:GLN:HG2	2:V:3:LEU:N	2.32	0.44
2:V:375:GLY:O	2:V:377:PHE:CD2	2.71	0.44
2:V:1068:GLN:C	2:V:1069:LEU:HG	2.37	0.44
1:A:183:TRP:CH2	1:A:374:HIS:CG	3.06	0.44
2:V:131:ILE:HG22	2:V:1058:THR:CG2	2.47	0.44
2:V:376:ASN:O	2:V:377:PHE:C	2.60	0.44
2:V:551:PRO:O	2:V:554:TYR:N	2.51	0.44
2:V:863:VAL:HG11	2:V:925:PRO:HA	1.99	0.44
2:V:902:PRO:HD2	2:V:905:PHE:CD2	2.53	0.44
2:V:1101:ASN:N	2:V:1101:ASN:HD22	2.14	0.44
2:V:1189:VAL:HG12	2:V:1191:LEU:N	2.33	0.44
2:V:1246:ARG:HD2	2:V:1247:TYR:CE2	2.52	0.44
1:A:205:TYR:HA	1:A:269:ILE:O	2.17	0.44
1:A:302:GLY:O	1:A:324:LYS:HA	2.17	0.44
2:V:252:ASN:O	2:V:254:TYR:CD1	2.67	0.44
2:V:1039:HIS:CE1	2:V:1081:SER:OG	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:448:VAL:HG12	2:V:449:GLU:N	2.33	0.44
2:V:1175:GLN:C	2:V:1176:ARG:CG	2.90	0.44
2:V:1323:ASN:ND2	2:V:1418:ILE:HG13	2.32	0.44
2:V:1355:TYR:CE1	2:V:1415:ASN:ND2	2.78	0.44
2:V:155:PHE:CE2	2:V:160:ILE:HD12	2.53	0.44
2:V:539:TYR:CD1	2:V:539:TYR:N	2.86	0.44
2:V:837:ASP:OD1	2:V:837:ASP:N	2.50	0.44
2:V:1358:THR:OG1	2:V:1413:THR:OG1	2.01	0.44
2:V:18:ASN:HA	2:V:19:PRO:HD3	1.83	0.44
2:V:346:ARG:N	9:V:2052:HOH:O	2.49	0.44
2:V:1374:LEU:HD12	2:V:1374:LEU:C	2.42	0.44
1:A:373:THR:HG22	1:A:374:HIS:H	1.83	0.43
2:V:259:ILE:HG21	2:V:267:VAL:HG11	1.99	0.43
2:V:368:VAL:HG21	2:V:385:TRP:CZ2	2.53	0.43
2:V:631:LEU:CA	2:V:654:ASP:O	2.66	0.43
2:V:896:SER:OG	2:V:909:ASP:HB3	2.18	0.43
2:V:1375:ASP:OD1	2:V:1376:VAL:N	2.51	0.43
1:A:334:MET:HE1	2:V:580:VAL:HB	1.99	0.43
2:V:13:GLU:OE1	2:V:40:ARG:NH2	2.51	0.43
2:V:345:ASP:HA	9:V:2052:HOH:O	2.17	0.43
2:V:545:ALA:O	2:V:546:VAL:C	2.61	0.43
2:V:1230:ASP:C	2:V:1230:ASP:OD1	2.61	0.43
2:V:1388:ILE:O	2:V:1389:ASN:CB	2.63	0.43
2:V:145:TYR:CZ	2:V:161:GLY:HA3	2.54	0.43
2:V:348:TYR:O	2:V:351:GLN:N	2.48	0.43
2:V:887:LEU:HB2	2:V:926:ARG:HH12	1.84	0.43
2:V:942:TYR:HB2	2:V:951:ILE:HG12	2.00	0.43
2:V:1286:ASN:HB2	2:V:1305:PHE:CG	2.53	0.43
2:V:1339:ILE:CD1	2:V:1407:ILE:CD1	2.61	0.43
2:V:119:GLN:HA	2:V:119:GLN:OE1	2.18	0.43
2:V:543:PRO:O	2:V:544:SER:C	2.62	0.43
2:V:1163:LYS:C	2:V:1165:HIS:N	2.76	0.43
2:V:631:LEU:N	2:V:631:LEU:CD2	2.81	0.43
2:V:1041:LEU:N	2:V:1041:LEU:CD1	2.81	0.43
2:V:1142:TRP:CH2	2:V:1188:THR:HG21	2.54	0.43
2:V:2:GLN:CG	2:V:3:LEU:N	2.81	0.43
2:V:90:ALA:CB	2:V:1056:GLY:C	2.91	0.43
2:V:133:PRO:HG3	2:V:141:LEU:HG	1.99	0.43
2:V:550:ASP:O	2:V:553:PHE:HB3	2.18	0.43
2:V:851:HIS:HB3	2:V:1026:GLN:O	2.18	0.43
2:V:882:HIS:ND1	2:V:883:ALA:N	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:946:ASN:N	2:V:950:ASP:OD2	2.51	0.43
2:V:1328:TRP:C	2:V:1328:TRP:HE3	2.26	0.43
2:V:108:VAL:HG21	2:V:1403:LEU:CB	2.49	0.43
2:V:196:ASN:O	2:V:198:TYR:N	2.52	0.43
2:V:239:ILE:O	2:V:239:ILE:HG13	2.16	0.43
2:V:275:ARG:NE	2:V:424:SER:O	2.52	0.43
2:V:357:SER:O	2:V:358:ASN:CB	2.66	0.43
2:V:799:TYR:CE2	2:V:836:ASP:HA	2.54	0.43
2:V:956:ILE:HG13	2:V:957:GLY:N	2.34	0.43
2:V:1102:GLN:O	2:V:1107:GLN:NE2	2.52	0.43
4:C:1:NAG:O4	4:C:2:NAG:H83	2.18	0.43
2:V:680:ILE:N	2:V:681:PRO:HD2	2.17	0.43
5:E:1:NAG:H61	5:E:1:NAG:O3	2.19	0.43
2:V:188:PHE:CZ	2:V:242:VAL:HG23	2.54	0.43
2:V:337:ALA:H	2:V:362:LYS:HG3	1.82	0.43
2:V:410:ASN:HB3	2:V:449:GLU:O	2.18	0.43
2:V:941:TYR:CD1	2:V:941:TYR:O	2.72	0.43
2:V:985:VAL:O	2:V:986:PHE:C	2.62	0.43
2:V:1038:TRP:HB2	2:V:1082:ILE:CG1	2.48	0.43
2:V:1255:PHE:CD1	2:V:1255:PHE:C	2.96	0.43
2:V:128:THR:CG2	2:V:129:ALA:H	2.29	0.43
2:V:862:GLU:O	2:V:865:ASP:HB2	2.19	0.43
2:V:1290:THR:HG22	2:V:1291:ALA:H	1.83	0.43
2:V:1383:VAL:HG23	2:V:1383:VAL:O	2.19	0.43
1:A:344:ASN:O	1:A:397:LYS:N	2.52	0.42
2:V:88:GLN:HG3	2:V:144:ALA:O	2.19	0.42
2:V:150:ASN:ND2	2:V:153:ARG:HB2	2.33	0.42
2:V:318:MET:O	2:V:319:LYS:CB	2.65	0.42
2:V:402:ASP:O	2:V:459:THR:HG23	2.18	0.42
2:V:419:TYR:O	2:V:478:TYR:CA	2.66	0.42
2:V:424:SER:HB2	2:V:461:LEU:CD1	2.48	0.42
2:V:880:SER:O	2:V:943:SER:HA	2.19	0.42
2:V:1138:HIS:ND1	2:V:1142:TRP:O	2.53	0.42
2:V:233:MET:HE2	2:V:264:GLY:HA2	2.00	0.42
2:V:255:LYS:C	2:V:256:VAL:HG13	2.45	0.42
2:V:867:ILE:O	2:V:920:VAL:HA	2.18	0.42
2:V:897:TYR:C	2:V:899:ASP:N	2.62	0.42
2:V:1036:VAL:HG12	2:V:1085:LYS:H	1.85	0.42
2:V:1149:LEU:HD11	2:V:1184:GLN:HB2	2.01	0.42
2:V:1302:TRP:CD1	2:V:1302:TRP:N	2.87	0.42
1:A:404:TRP:O	1:A:408:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:3:LEU:CD1	2:V:72:ILE:HD13	2.33	0.42
2:V:412:ALA:HB3	2:V:416:TYR:HE2	1.84	0.42
2:V:502:LYS:O	2:V:504:LEU:N	2.51	0.42
2:V:882:HIS:ND1	2:V:882:HIS:C	2.77	0.42
2:V:913:PRO:C	2:V:915:GLY:N	2.77	0.42
2:V:1208:GLY:HA2	2:V:1247:TYR:CE2	2.54	0.42
2:V:1294:TYR:CB	2:V:1304:PRO:HD3	2.44	0.42
2:V:1318:TRP:CE3	2:V:1318:TRP:O	2.72	0.42
1:A:180:GLU:C	1:A:182:PRO:HD3	2.44	0.42
2:V:848:TYR:C	2:V:850:LYS:N	2.75	0.42
1:A:335:VAL:HA	2:V:512:LYS:HD3	2.01	0.42
2:V:250:GLU:HB3	2:V:270:ASP:OD1	2.19	0.42
2:V:450:PRO:C	2:V:452:GLN:H	2.28	0.42
2:V:478:TYR:CE1	2:V:494:GLY:HA3	2.55	0.42
2:V:639:TRP:O	2:V:639:TRP:CD2	2.72	0.42
2:V:926:ARG:C	2:V:926:ARG:HD2	2.44	0.42
2:V:346:ARG:C	2:V:348:TYR:H	2.28	0.42
2:V:410:ASN:OD1	2:V:411:LEU:N	2.53	0.42
2:V:523:VAL:O	2:V:523:VAL:HG12	2.19	0.42
2:V:542:ASN:OD1	2:V:542:ASN:N	2.52	0.42
2:V:808:ASP:CB	2:V:825:THR:CA	2.95	0.42
2:V:939:TRP:O	2:V:959:ILE:HB	2.19	0.42
2:V:1370:TRP:CH2	2:V:1408:ARG:HG3	2.53	0.42
2:V:801:ALA:HB3	2:V:834:TYR:HE2	1.85	0.42
2:V:906:LYS:O	2:V:909:ASP:HB2	2.20	0.42
2:V:1028:LEU:CD2	2:V:1094:LEU:HD11	2.49	0.42
2:V:1188:THR:O	2:V:1194:HIS:O	2.38	0.42
1:A:118:GLY:CA	1:A:124:CYS:H	2.32	0.42
1:A:175:ASP:HA	1:A:321:LYS:HA	2.00	0.42
2:V:180:PHE:HD1	2:V:225:HIS:ND1	2.17	0.42
2:V:422:GLY:HA3	2:V:476:LYS:CE	2.49	0.42
2:V:548:LYS:O	2:V:549:ASP:CG	2.63	0.42
2:V:800:ILE:HG21	2:V:831:PHE:HD2	1.84	0.42
2:V:1370:TRP:CZ3	2:V:1408:ARG:HG3	2.54	0.42
2:V:86:HIS:HA	2:V:87:PRO:HD3	1.81	0.42
2:V:448:VAL:HG21	2:V:454:TYR:HB3	2.02	0.42
2:V:1185:THR:HG22	2:V:1186:GLN:N	2.35	0.42
1:A:264:TYR:HD1	1:A:401:PHE:CE2	2.38	0.42
2:V:42:TYR:CD1	2:V:49:GLU:CG	3.03	0.42
2:V:300:LYS:HB2	2:V:300:LYS:HE2	1.81	0.42
2:V:408:PHE:N	2:V:454:TYR:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:131:ILE:O	2:V:131:ILE:CD1	2.65	0.41
2:V:188:PHE:CZ	2:V:242:VAL:CG2	3.03	0.41
2:V:188:PHE:HB3	2:V:240:PHE:CE2	2.55	0.41
2:V:528:LYS:CE	2:V:590:THR:HG21	2.49	0.41
2:V:1021:ILE:HG21	2:V:1025:LEU:N	2.34	0.41
2:V:1105:GLY:O	2:V:1107:GLN:N	2.53	0.41
2:V:1111:THR:CG2	2:V:1112:VAL:N	2.81	0.41
2:V:48:GLN:O	2:V:48:GLN:CD	2.52	0.41
2:V:212:ASN:ND2	4:C:1:NAG:HO6	2.14	0.41
2:V:287:LYS:O	2:V:290:GLN:HG2	2.20	0.41
2:V:497:LEU:HD11	2:V:518:HIS:CE1	2.56	0.41
2:V:523:VAL:HG23	2:V:648:MET:HE1	2.02	0.41
2:V:885:GLY:HA3	2:V:939:TRP:CE3	2.55	0.41
2:V:911:ILE:HD13	2:V:917:TYR:HB2	2.01	0.41
1:A:202:SER:CB	1:A:203:PRO:CD	2.98	0.41
1:A:410:ARG:NH1	1:A:410:ARG:CG	2.72	0.41
2:V:240:PHE:N	2:V:240:PHE:CD1	2.88	0.41
2:V:260:ASN:HB3	2:V:617:PHE:CG	2.55	0.41
2:V:348:TYR:HE2	2:V:646:ASN:HB2	1.78	0.41
2:V:573:LEU:O	2:V:652:PHE:HB2	2.20	0.41
2:V:854:ILE:HG23	2:V:855:LEU:N	2.35	0.41
2:V:908:ASP:HB3	2:V:917:TYR:CZ	2.56	0.41
2:V:1407:ILE:HD12	2:V:1424:LEU:CD1	2.50	0.41
2:V:17:TYR:HD2	2:V:211:ALA:HB2	1.85	0.41
2:V:50:LYS:CB	2:V:51:PRO:HD2	2.47	0.41
2:V:203:LEU:HD12	2:V:203:LEU:C	2.45	0.41
2:V:261:LEU:HD23	2:V:261:LEU:N	2.28	0.41
2:V:327:ILE:HA	2:V:370:ARG:O	2.21	0.41
2:V:588:VAL:O	2:V:591:VAL:HG23	2.21	0.41
2:V:1222:GLN:CG	2:V:1223:MET:N	2.83	0.41
2:V:1360:SER:O	2:V:1361:ILE:HG13	2.19	0.41
1:A:400:LYS:NZ	2:V:657:TYR:CZ	2.86	0.41
2:V:16:ASP:C	2:V:18:ASN:N	2.77	0.41
2:V:519:ALA:HB2	2:V:583:TRP:HZ3	1.85	0.41
2:V:582:GLN:HE21	2:V:625:THR:HG22	1.85	0.41
2:V:1360:SER:C	2:V:1361:ILE:HG13	2.45	0.41
2:V:137:ASP:HB3	2:V:138:PRO:HD2	2.02	0.41
2:V:600:SER:HB3	2:V:634:TRP:CE3	2.55	0.41
2:V:886:LEU:CD2	2:V:923:VAL:HG22	2.51	0.41
2:V:939:TRP:O	2:V:959:ILE:N	2.51	0.41
2:V:1032:LYS:HD2	2:V:1089:ILE:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:1230:ASP:OD1	2:V:1233:THR:N	2.47	0.41
2:V:1389:ASN:CG	2:V:1390:SER:N	2.76	0.41
2:V:368:VAL:HG12	2:V:391:ILE:HD11	2.02	0.41
2:V:396:ILE:CG2	2:V:397:LYS:H	2.32	0.41
2:V:634:TRP:HB2	2:V:652:PHE:CE1	2.56	0.41
2:V:942:TYR:CE2	2:V:951:ILE:HD11	2.52	0.41
2:V:1050:HIS:O	2:V:1052:VAL:N	2.54	0.41
2:V:1324:ASN:C	2:V:1326:ASP:H	2.27	0.41
2:V:1344:THR:C	2:V:1387:ASN:HD21	2.29	0.41
1:A:369:VAL:HG12	1:A:370:TYR:N	2.35	0.41
2:V:96:SER:N	2:V:112:ASP:OD2	2.50	0.41
2:V:122:LYS:HB3	2:V:122:LYS:HE3	1.82	0.41
2:V:142:THR:CG2	2:V:231:ILE:HD11	2.51	0.41
2:V:331:GLU:OE2	2:V:413:SER:CB	2.69	0.41
2:V:334:TRP:NE1	2:V:336:TYR:CD1	2.87	0.41
2:V:419:TYR:O	2:V:478:TYR:HB2	2.20	0.41
2:V:497:LEU:CD1	2:V:518:HIS:HE1	2.33	0.41
2:V:599:LEU:O	2:V:600:SER:CB	2.64	0.41
2:V:887:LEU:HB2	2:V:924:PRO:HG3	2.03	0.41
2:V:1149:LEU:O	2:V:1150:ASN:HB2	2.20	0.41
1:A:257:PHE:O	1:A:258:ASP:C	2.61	0.41
2:V:81:GLN:OE1	2:V:82:PRO:HD3	2.21	0.41
2:V:86:HIS:NE2	2:V:1055:HIS:CE1	2.83	0.41
2:V:210:PHE:HD1	9:V:2004:HOH:O	2.03	0.41
2:V:228:TRP:CD1	2:V:271:MET:HE3	2.41	0.41
2:V:240:PHE:CB	2:V:261:LEU:HD21	2.46	0.41
2:V:245:ASN:O	2:V:246:GLY:C	2.64	0.41
2:V:254:TYR:CE2	2:V:607:LYS:HE3	2.55	0.41
2:V:629:ASP:OD2	2:V:926:ARG:NH2	2.54	0.41
2:V:639:TRP:HH2	2:V:1043:MET:O	2.03	0.41
2:V:678:ILE:HG22	2:V:679:PHE:H	1.86	0.41
2:V:894:GLY:O	2:V:944:GLY:HA3	2.21	0.41
2:V:993:TYR:O	2:V:994:PHE:HB2	2.20	0.41
2:V:1042:ASN:OD1	2:V:1042:ASN:C	2.64	0.41
2:V:1367:ASN:O	2:V:1369:THR:N	2.54	0.41
1:A:176:CYS:O	1:A:177:LYS:C	2.63	0.41
2:V:77:ASN:OD1	2:V:79:ALA:HB3	2.21	0.41
2:V:1021:ILE:HD12	2:V:1025:LEU:HD13	2.02	0.41
2:V:1030:MET:CE	2:V:1110:PHE:HB2	2.50	0.41
2:V:1201:PHE:HB2	2:V:1223:MET:O	2.21	0.41
2:V:150:ASN:ND2	2:V:153:ARG:HG2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:636:LEU:C	2:V:636:LEU:CD2	2.92	0.40
2:V:823:LYS:O	2:V:824:THR:CB	2.69	0.40
2:V:860:ARG:HA	2:V:960:LEU:O	2.21	0.40
2:V:1151:ASN:ND2	2:V:1152:THR:O	2.54	0.40
2:V:1282:GLY:O	2:V:1283:ALA:C	2.64	0.40
2:V:1420:LEU:C	2:V:1420:LEU:CD1	2.94	0.40
2:V:155:PHE:HD1	2:V:156:ASN:H	1.59	0.40
2:V:849:GLU:HG3	2:V:852:LEU:HD11	2.02	0.40
2:V:911:ILE:CD1	2:V:917:TYR:CB	2.94	0.40
1:A:116:LEU:O	1:A:124:CYS:HA	2.21	0.40
2:V:144:ALA:CB	2:V:233:MET:HE1	2.52	0.40
2:V:348:TYR:CD2	2:V:646:ASN:ND2	2.71	0.40
2:V:888:TYR:HB3	2:V:921:TRP:HD1	1.78	0.40
2:V:1036:VAL:CG1	2:V:1084:MET:HB3	2.47	0.40
1:A:347:CYS:HA	1:A:393:GLY:O	2.22	0.40
2:V:115:VAL:HG13	2:V:119:GLN:HB2	2.03	0.40
2:V:156:ASN:HB2	9:V:2031:HOH:O	2.21	0.40
2:V:528:LYS:HE3	2:V:590:THR:HG21	2.03	0.40
2:V:654:ASP:OD1	2:V:654:ASP:C	2.64	0.40
2:V:952:HIS:HD2	2:V:987:ASP:N	2.18	0.40
2:V:1036:VAL:O	2:V:1084:MET:N	2.48	0.40
2:V:1078:THR:HG22	2:V:1079:PHE:N	2.35	0.40
1:A:242:ILE:N	2:V:679:PHE:O	2.55	0.40
2:V:233:MET:HE3	2:V:233:MET:HB2	1.85	0.40
2:V:639:TRP:O	2:V:639:TRP:CE3	2.74	0.40
2:V:914:ASN:O	2:V:915:GLY:C	2.64	0.40
2:V:943:SER:OG	2:V:955:LEU:CD2	2.66	0.40
2:V:1049:ILE:O	2:V:1050:HIS:CD2	2.74	0.40
2:V:1052:VAL:HA	2:V:1095:GLU:O	2.21	0.40
2:V:1117:CYS:SG	2:V:1117:CYS:O	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	232/423 (55%)	195 (84%)	27 (12%)	10 (4%)	2	15
2	V	1243/1430 (87%)	961 (77%)	196 (16%)	86 (7%)	1	7
All	All	1475/1853 (80%)	1156 (78%)	223 (15%)	96 (6%)	1	8

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ILE
1	A	305	SER
1	A	410	ARG
2	V	52	ARG
2	V	66	GLU
2	V	151	MET
2	V	257	SER
2	V	344	VAL
2	V	349	LYS
2	V	484	MET
2	V	500	LYS
2	V	551	PRO
2	V	659	ASP
2	V	680	ILE
2	V	682	SER
2	V	796	ARG
2	V	832	ARG
2	V	898	ASP
2	V	971	ASN
2	V	1024	GLN
2	V	1107	GLN
2	V	1127	ILE
2	V	1191	LEU
2	V	1317	ALA
2	V	1368	SER
2	V	1389	ASN
1	A	136	ILE
1	A	175	ASP
1	A	184	GLN
1	A	397	LYS
2	V	156	ASN
2	V	174	ASN
2	V	197	TRP

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Mol	Chain	Res	Type
2	V	256	VAL
2	V	386	PRO
2	V	388	GLU
2	V	503	ALA
2	V	515	VAL
2	V	600	SER
2	V	601	GLY
2	V	607	LYS
2	V	669	GLU
2	V	675	PHE
2	V	874	LEU
2	V	1023	TYR
2	V	1026	GLN
2	V	1051	VAL
2	V	1062	GLU
2	V	1106	MET
2	V	1257	ASN
2	V	1293	SER
2	V	1394	VAL
2	V	1399	LYS
2	V	11	GLN
2	V	43	GLU
2	V	284	LEU
2	V	338	PRO
2	V	527	ASN
2	V	552	LYS
2	V	795	LYS
2	V	964	LYS
2	V	969	LYS
2	V	1016	PRO
2	V	1274	SER
2	V	1418	ILE
1	A	124	CYS
2	V	60	GLY
2	V	69	ASP
2	V	146	TYR
2	V	166	CYS
2	V	357	SER
2	V	512	LYS
2	V	656	ASN
2	V	679	PHE
2	V	849	GLU

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Mol	Chain	Res	Type
2	V	855	LEU
2	V	1165	HIS
2	V	1352	THR
2	V	1401	PRO
1	A	411	GLN
2	V	19	PRO
2	V	274	SER
2	V	343	SER
2	V	1129	GLN
1	A	122	HIS
2	V	549	ASP
2	V	947	PRO
2	V	1025	LEU
2	V	1045	GLY
2	V	546	VAL
2	V	913	PRO
2	V	127	ILE
2	V	945	VAL
2	V	994	PHE
2	V	237	PRO
2	V	588	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	111/368 (30%)	106 (96%)	5 (4%)	24	53
2	V	878/1260 (70%)	786 (90%)	92 (10%)	6	25
All	All	989/1628 (61%)	892 (90%)	97 (10%)	7	28

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	174	MET

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Mol	Chain	Res	Type
1	A	255	TYR
1	A	341	ILE
1	A	407	ARG
2	V	48	GLN
2	V	64	ARG
2	V	80	THR
2	V	131	ILE
2	V	150	ASN
2	V	151	MET
2	V	155	PHE
2	V	163	LEU
2	V	172	ASN
2	V	174	ASN
2	V	181	ASN
2	V	199	ARG
2	V	200	LYS
2	V	230	LEU
2	V	252	ASN
2	V	276	THR
2	V	289	LEU
2	V	346	ARG
2	V	355	ASN
2	V	362	LYS
2	V	364	TYR
2	V	452	GLN
2	V	468	VAL
2	V	484	MET
2	V	485	THR
2	V	511	ASN
2	V	512	LYS
2	V	514	ASP
2	V	527	ASN
2	V	549	ASP
2	V	558	VAL
2	V	561	THR
2	V	562	LEU
2	V	581	VAL
2	V	585	LEU
2	V	592	ASP
2	V	611	GLN
2	V	626	VAL
2	V	631	LEU

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Mol	Chain	Res	Type
2	V	657	TYR
2	V	800	ILE
2	V	809	TYR
2	V	874	LEU
2	V	877	ARG
2	V	926	ARG
2	V	931	ASP
2	V	943	SER
2	V	972	ARG
2	V	973	THR
2	V	977	ARG
2	V	984	MET
2	V	993	TYR
2	V	1013	HIS
2	V	1018	ILE
2	V	1030	MET
2	V	1034	GLU
2	V	1042	ASN
2	V	1057	GLN
2	V	1058	THR
2	V	1069	LEU
2	V	1079	PHE
2	V	1094	LEU
2	V	1101	ASN
2	V	1102	GLN
2	V	1111	THR
2	V	1119	LEU
2	V	1120	PRO
2	V	1141	TYR
2	V	1151	ASN
2	V	1156	ASN
2	V	1176	ARG
2	V	1211	TRP
2	V	1236	GLU
2	V	1246	ARG
2	V	1257	ASN
2	V	1258	ARG
2	V	1260	THR
2	V	1261	PHE
2	V	1271	GLU
2	V	1286	ASN
2	V	1288	GLU

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Mol	Chain	Res	Type
2	V	1299	TRP
2	V	1309	LEU
2	V	1335	HIS
2	V	1336	LEU
2	V	1344	THR
2	V	1348	THR
2	V	1354	MET
2	V	1364	THR
2	V	1384	PHE
2	V	1389	ASN
2	V	1427	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	344	ASN
2	V	7	HIS
2	V	11	GLN
2	V	20	GLN
2	V	48	GLN
2	V	86	HIS
2	V	148	HIS
2	V	150	ASN
2	V	156	ASN
2	V	174	ASN
2	V	260	ASN
2	V	288	HIS
2	V	290	GLN
2	V	371	GLN
2	V	479	HIS
2	V	501	HIS
2	V	511	ASN
2	V	517	GLN
2	V	527	ASN
2	V	576	HIS
2	V	577	GLN
2	V	582	GLN
2	V	598	HIS
2	V	922	GLN
2	V	952	HIS
2	V	1037	HIS

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Mol	Chain	Res	Type
2	V	1055	HIS
2	V	1057	GLN
2	V	1067	ASN
2	V	1101	ASN
2	V	1107	GLN
2	V	1151	ASN
2	V	1156	ASN
2	V	1177	GLN
2	V	1184	GLN
2	V	1222	GLN
2	V	1224	HIS
2	V	1257	ASN
2	V	1286	ASN
2	V	1319	GLN
2	V	1323	ASN
2	V	1362	HIS
2	V	1393	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	B	1	3,2	14,14,15	0.82	0	17,19,21	1.41	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FUC	B	2	3	10,10,11	0.71	0	14,14,16	0.63	0
4	NAG	C	1	4,2	14,14,15	0.50	0	17,19,21	0.77	0
4	NAG	C	2	4	14,14,15	0.53	0	17,19,21	0.81	1 (5%)
4	BMA	C	3	4	11,11,12	0.30	0	15,15,17	0.67	0
4	MAN	C	4	4	11,11,12	0.62	0	15,15,17	0.53	0
4	MAN	C	5	4	11,11,12	0.68	0	15,15,17	0.65	0
4	MAN	C	6	4	11,11,12	0.61	0	15,15,17	0.72	0
4	MAN	C	7	4	11,11,12	0.69	0	15,15,17	0.68	0
4	MAN	C	8	4	11,11,12	0.64	0	15,15,17	0.55	0
5	NAG	D	1	5,2	14,14,15	0.56	0	17,19,21	0.80	0
5	NAG	D	2	5	11,11,15	0.62	0	13,15,21	0.62	0
5	NAG	E	1	5,2	14,14,15	0.61	0	17,19,21	0.71	0
5	NAG	E	2	5	14,14,15	0.54	0	17,19,21	0.74	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
3	NAG	B	1	3,2	-	5/6/23/26	0/1/1/1
3	FUC	B	2	3	-	-	0/1/1/1
4	NAG	C	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	C	2	4	-	2/6/23/26	0/1/1/1
4	BMA	C	3	4	-	2/2/19/22	0/1/1/1
4	MAN	C	4	4	-	2/2/19/22	0/1/1/1
4	MAN	C	5	4	-	2/2/19/22	0/1/1/1
4	MAN	C	6	4	-	0/2/19/22	0/1/1/1
4	MAN	C	7	4	-	2/2/19/22	0/1/1/1
4	MAN	C	8	4	-	0/2/19/22	0/1/1/1
5	NAG	D	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	D	2	5	-	2/2/19/26	0/1/1/1
5	NAG	E	1	5,2	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	E	2	5	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	NAG	O5-C1-C2	-3.15	106.42	111.29
3	B	1	NAG	C4-C3-C2	2.69	114.96	111.02
3	B	1	NAG	O5-C5-C4	-2.27	105.30	110.83
3	B	1	NAG	C2-N2-C7	2.17	125.80	122.90
4	C	2	NAG	O5-C1-C2	-2.17	107.94	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	1	NAG	C1

All (27) torsion outliers are listed below:

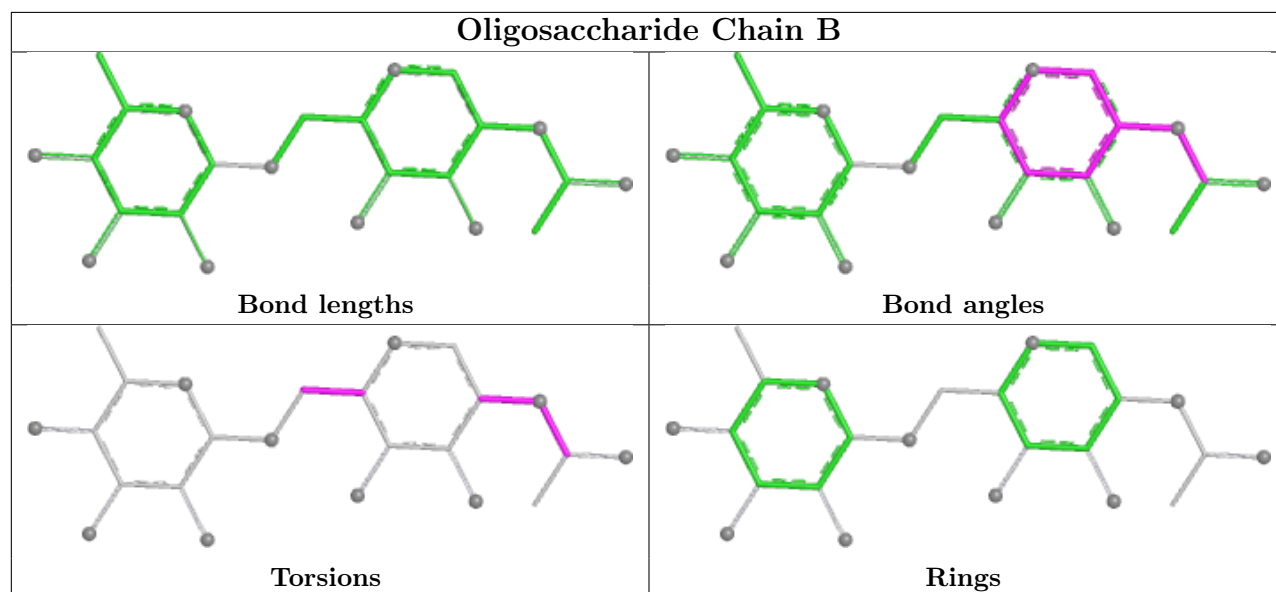
Mol	Chain	Res	Type	Atoms
3	B	1	NAG	C1-C2-N2-C7
5	E	2	NAG	C3-C2-N2-C7
4	C	3	BMA	C4-C5-C6-O6
4	C	5	MAN	O5-C5-C6-O6
5	D	2	NAG	O5-C5-C6-O6
3	B	1	NAG	O5-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	C	5	MAN	C4-C5-C6-O6
5	D	2	NAG	C4-C5-C6-O6
4	C	3	BMA	O5-C5-C6-O6
4	C	7	MAN	O5-C5-C6-O6
5	D	1	NAG	O5-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6
5	D	1	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
3	B	1	NAG	C8-C7-N2-C2
3	B	1	NAG	O7-C7-N2-C2
4	C	2	NAG	C8-C7-N2-C2
4	C	2	NAG	O7-C7-N2-C2
4	C	4	MAN	C4-C5-C6-O6
4	C	7	MAN	C4-C5-C6-O6
4	C	4	MAN	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
3	B	1	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	E	1	NAG	C3-C2-N2-C7

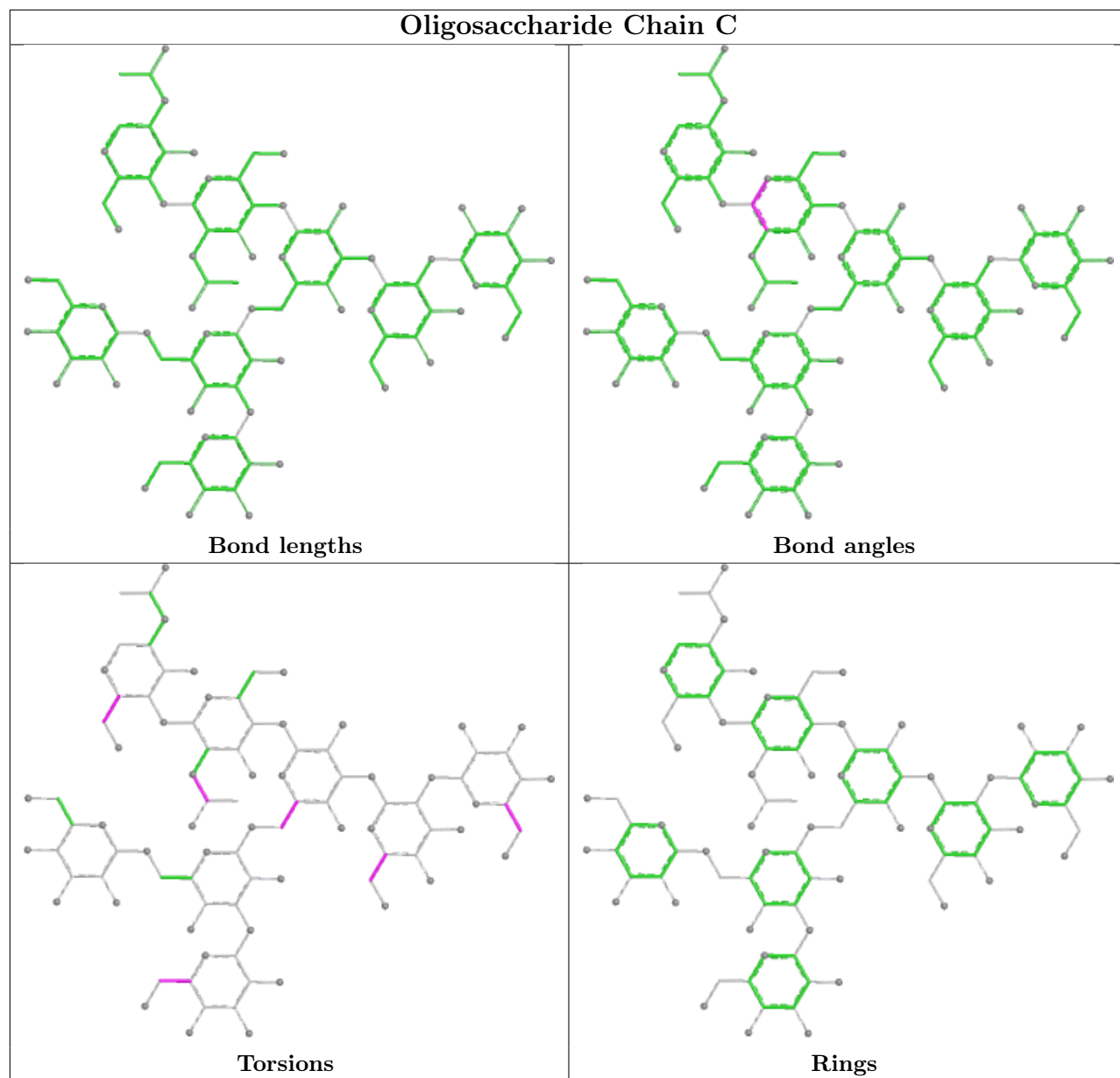
There are no ring outliers.

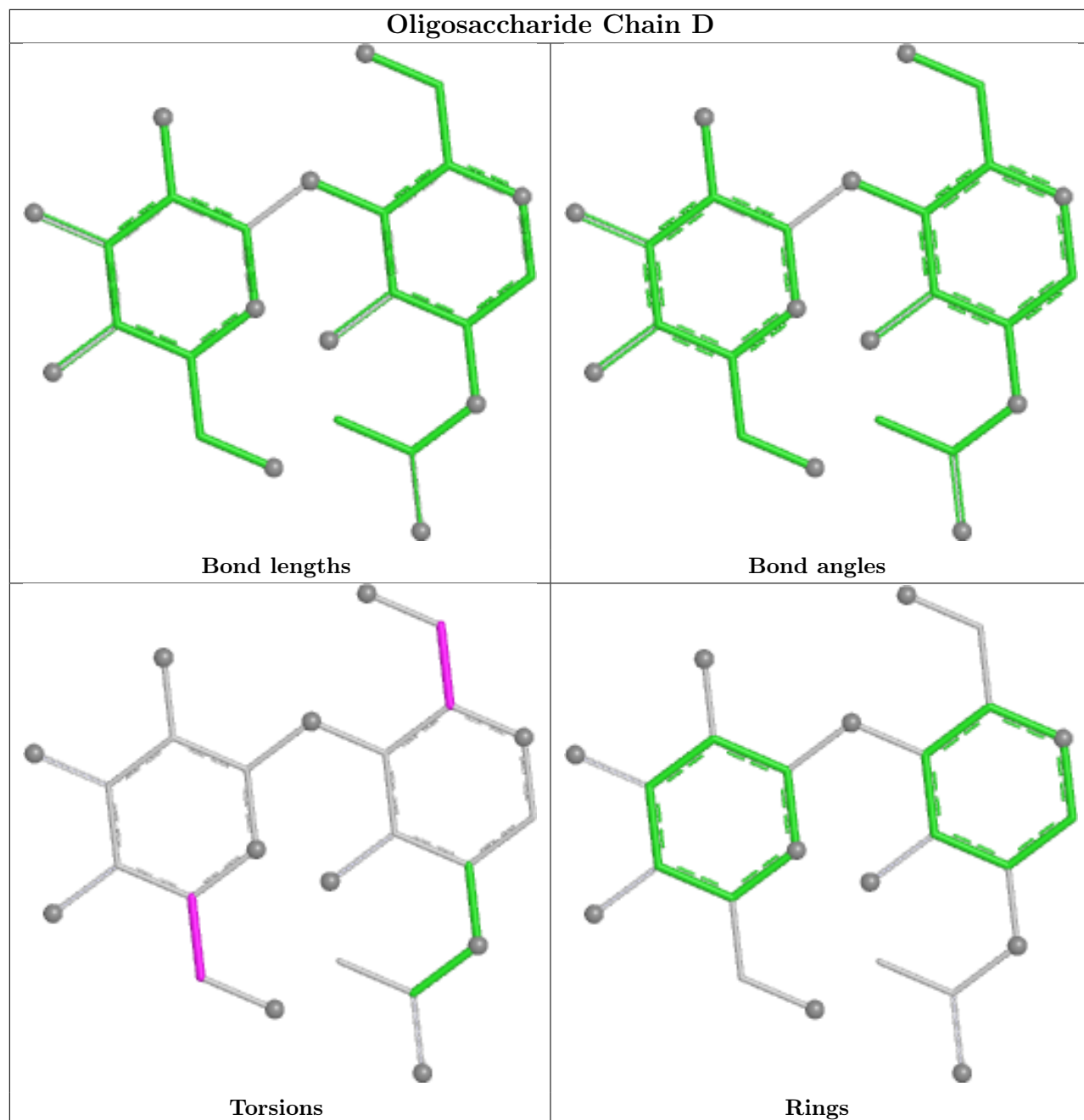
9 monomers are involved in 18 short contacts:

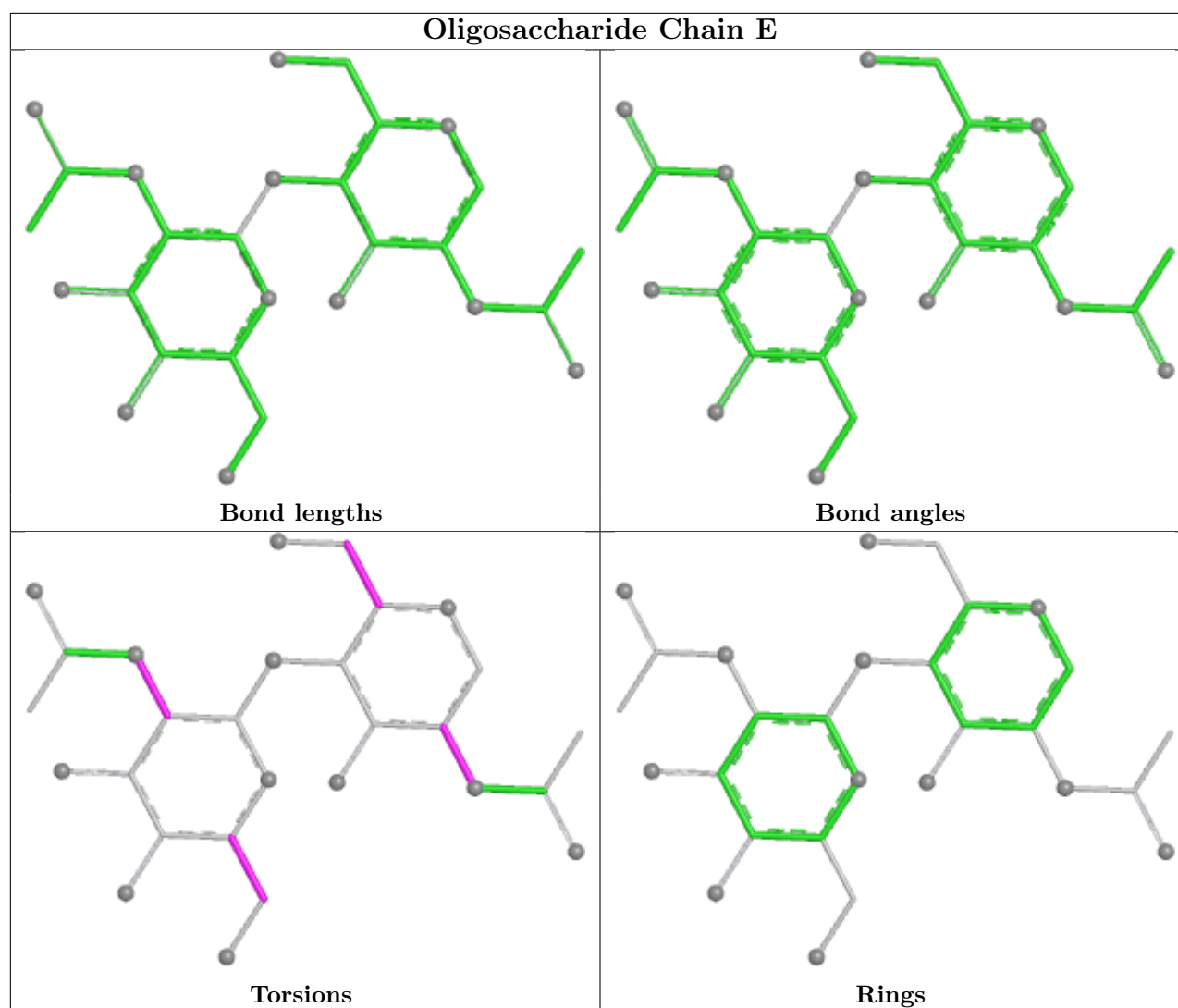
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	4	MAN	2	0
4	C	3	BMA	1	0
3	B	1	NAG	4	0
4	C	6	MAN	1	0
5	E	1	NAG	1	0
5	E	2	NAG	2	0
4	C	8	MAN	1	0
4	C	1	NAG	6	0
4	C	2	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
6	NAG	V	1521	2	14,14,15	0.52	0	17,19,21	0.73	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
6	NAG	V	1521	2	1/1/5/7	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	V	1521	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	V	1521	NAG	C8-C7-N2-C2
6	V	1521	NAG	O7-C7-N2-C2
6	V	1521	NAG	O5-C5-C6-O6
6	V	1521	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	V	1521	NAG	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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	248/423 (58%)	0.61	21 (8%)	16 13	82, 154, 205, 249	0
2	V	1249/1430 (87%)	0.45	64 (5%)	33 22	65, 122, 172, 255	0
All	All	1497/1853 (80%)	0.48	85 (5%)	29 20	65, 126, 185, 255	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	1119	LEU	4.4
1	A	87	LYS	4.2
2	V	885	GLY	4.1
2	V	639	TRP	3.9
2	V	1121	MET	3.8
1	A	307	PHE	3.8
2	V	385	TRP	3.7
1	A	212	CYS	3.6
2	V	1185	THR	3.5
1	A	368	THR	3.4
2	V	388	GLU	3.3
1	A	361	ASP	3.1
2	V	939	TRP	3.1
1	A	284	ALA	3.0
2	V	444	HIS	2.9
2	V	646	ASN	2.8
2	V	1038	TRP	2.7
2	V	434	TYR	2.7
2	V	1174	LEU	2.7
2	V	1263	ILE	2.7
2	V	798	TYR	2.7
2	V	1300	SER	2.6
2	V	1321	GLU	2.6
1	A	374	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
2	V	201	PRO	2.5
2	V	1245	ALA	2.5
1	A	266	ILE	2.5
2	V	943	SER	2.5
1	A	225	GLU	2.5
2	V	306	ASP	2.5
2	V	1358	THR	2.5
1	A	383	GLY	2.5
2	V	927	SER	2.4
2	V	1201	PHE	2.4
2	V	920	VAL	2.4
2	V	1419	ALA	2.4
2	V	1350	MET	2.4
2	V	345	ASP	2.4
1	A	395	TYR	2.4
1	A	296	LEU	2.4
2	V	871	PHE	2.4
2	V	845	GLY	2.3
2	V	940	ALA	2.3
2	V	898	ASP	2.3
2	V	1261	PHE	2.3
2	V	284	LEU	2.3
1	A	185	ALA	2.3
2	V	517	GLN	2.3
2	V	922	GLN	2.3
2	V	430	GLU	2.3
1	A	398	LEU	2.3
1	A	211	HIS	2.3
2	V	638	SER	2.3
1	A	304	VAL	2.3
2	V	489	ALA	2.2
2	V	1298	TRP	2.2
2	V	880	SER	2.2
1	A	130	PHE	2.2
1	A	277	PHE	2.2
2	V	900	LYS	2.2
2	V	1305	PHE	2.2
2	V	1188	THR	2.2
1	A	394	ASN	2.2
2	V	1065	GLU	2.2
2	V	657	TYR	2.1
2	V	249	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	V	1094	LEU	2.1
2	V	35	LYS	2.1
2	V	179	PHE	2.1
2	V	455	THR	2.1
2	V	384	ILE	2.1
2	V	500	LYS	2.1
2	V	910	ALA	2.1
2	V	1029	THR	2.1
2	V	559	MET	2.1
1	A	348	ALA	2.1
1	A	326	PRO	2.1
2	V	1259	PRO	2.1
2	V	343	SER	2.0
2	V	505	SER	2.0
2	V	266	SER	2.0
2	V	265	ALA	2.0
2	V	503	ALA	2.0
2	V	169	GLY	2.0
2	V	1077	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

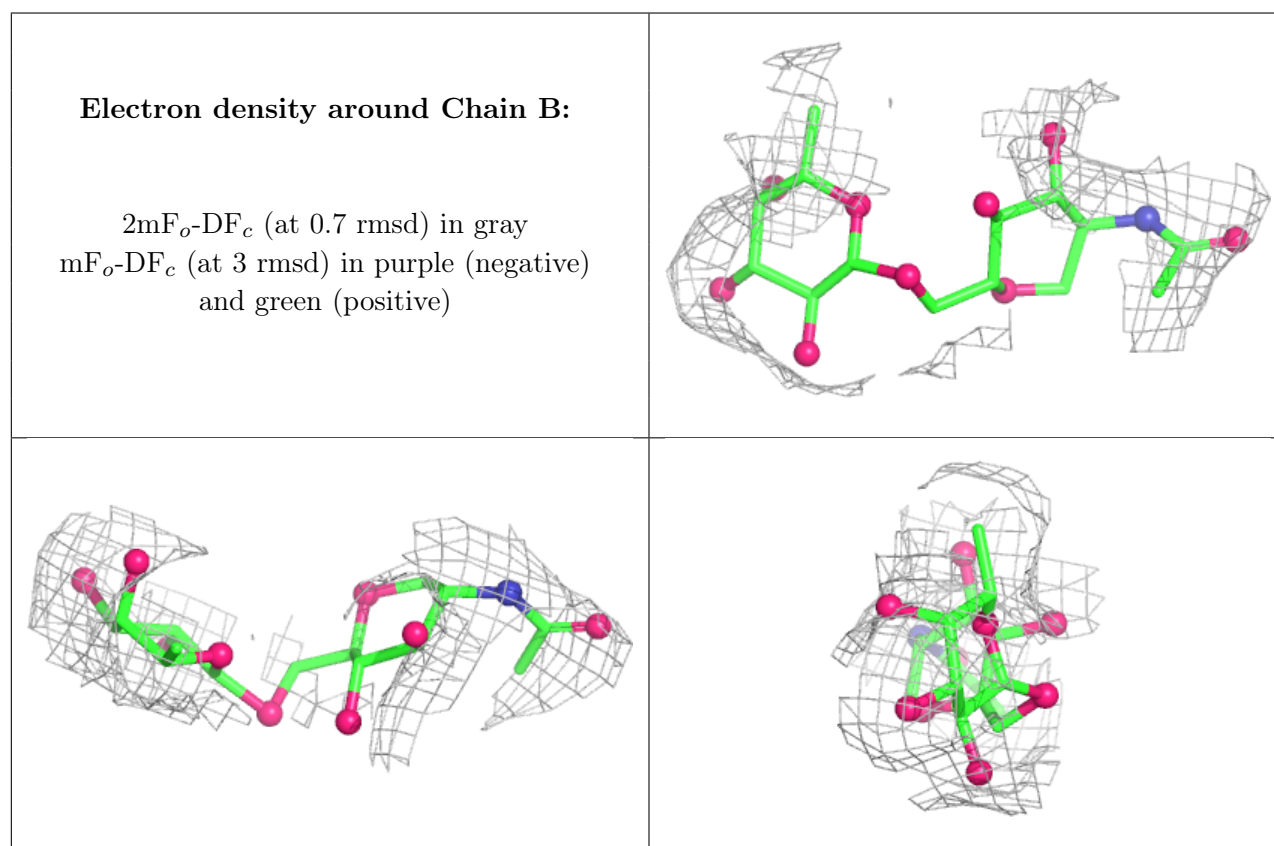
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	1	14/15	-	-	170,211,254,267	0
3	FUC	B	2	10/11	-	-	174,220,248,281	0
5	NAG	E	2	14/15	0.39	0.12	166,195,234,249	0
4	NAG	C	2	14/15	-	-	100,114,135,135	0
4	BMA	C	3	11/12	-	-	120,126,151,159	0
4	MAN	C	4	11/12	-	-	122,131,153,163	0
4	MAN	C	5	11/12	-	-	124,154,178,181	0
4	MAN	C	6	11/12	-	-	89,146,182,203	0
4	MAN	C	7	11/12	-	-	99,147,176,234	0

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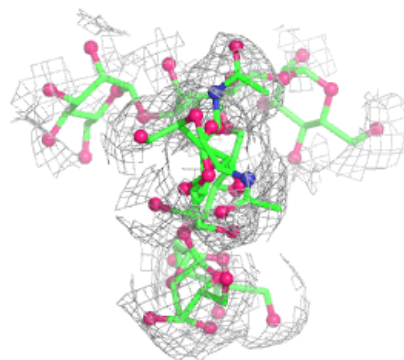
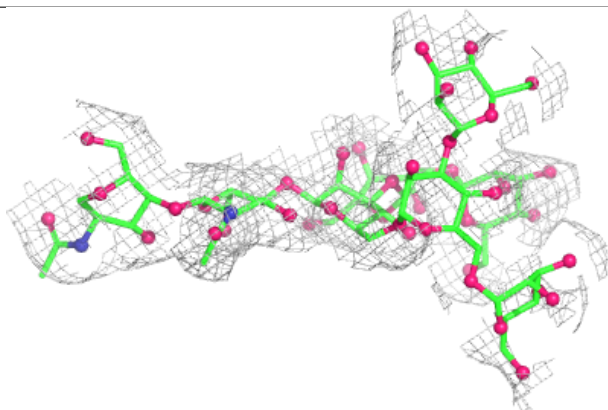
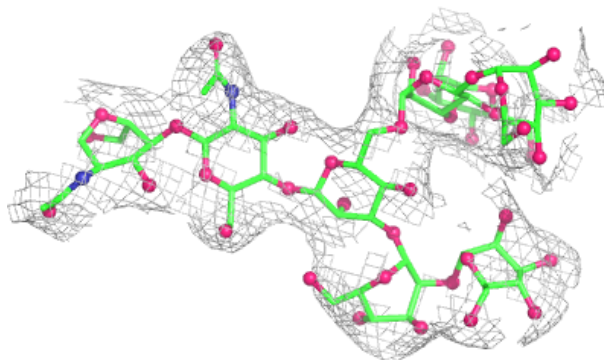
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MAN	C	8	11/12	-	-	166,216,232,241	0
4	NAG	C	1	14/15	0.50	0.11	109,122,134,138	0
5	NAG	D	1	14/15	0.89	0.09	123,145,212,220	0
5	NAG	D	2	11/15	0.91	0.10	171,180,203,215	0
5	NAG	E	1	14/15	0.92	0.12	132,201,219,237	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

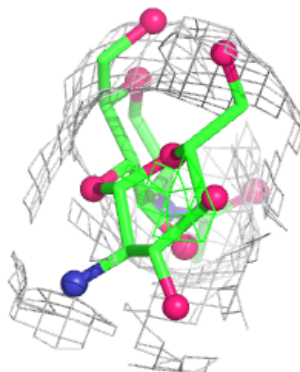
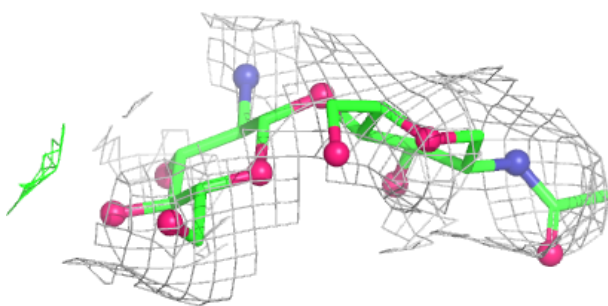
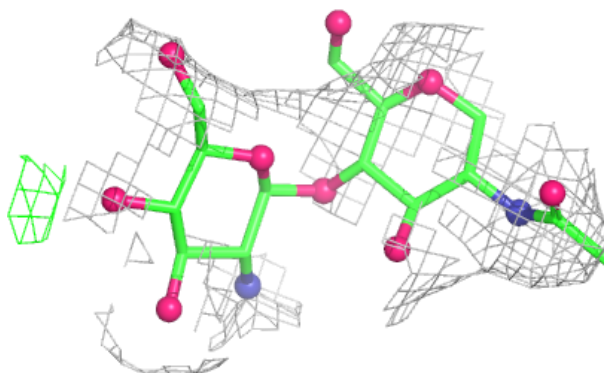


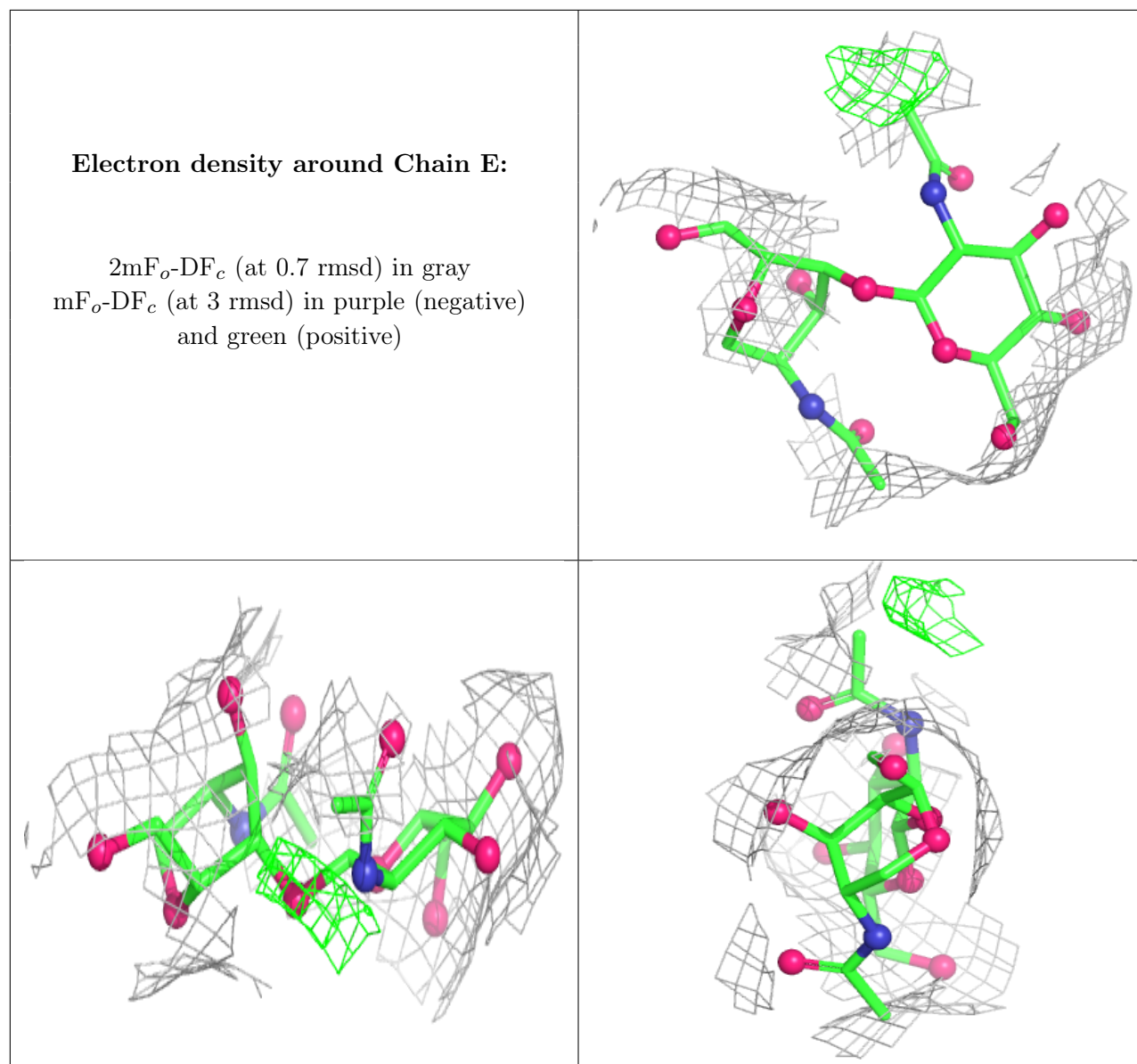
Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain D:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	V	1521	14/15	0.52	0.13	152,206,263,286	0
8	CU	V	2432	1/1	0.97	0.05	124,124,124,124	0
7	CA	V	2431	1/1	0.99	0.06	105,105,105,105	0
7	CA	V	2430	1/1	0.99	0.03	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.