



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:13 AM UTC

PDB ID : 3R05 / pdb_00003r05
Title : Structure of neurexin 1 alpha (domains LNS1-LNS6), with splice insert SS3
Authors : Venugopal, V.; Rudenko, G.
Deposited on : 2011-03-07
Resolution : 2.95 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

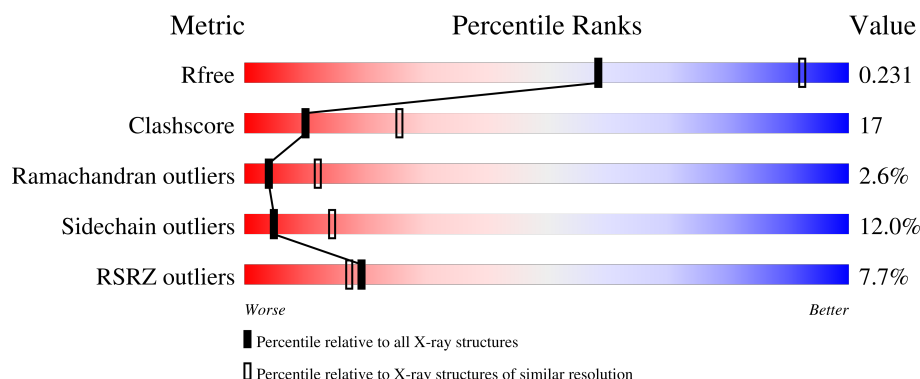
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	1254	7% 46% 27% 6% • 20%
1	B	1254	6% 45% 27% 7% • 20%
2	C	2	100%
2	D	2	50% 50%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15522 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 Neurexin-1-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1008	Total	C	N	O	S	0	0	0
			7733	4857	1334	1499	43			
1	B	1008	Total	C	N	O	S	0	0	0
			7733	4857	1334	1499	43			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1340	ALA	-	expression tag	UNP Q28146
A	1341	SER	-	expression tag	UNP Q28146
A	1342	THR	-	expression tag	UNP Q28146
A	1343	SER	-	expression tag	UNP Q28146
A	1344	HIS	-	expression tag	UNP Q28146
A	1345	HIS	-	expression tag	UNP Q28146
A	1346	HIS	-	expression tag	UNP Q28146
A	1347	HIS	-	expression tag	UNP Q28146
A	1348	HIS	-	expression tag	UNP Q28146
A	1349	HIS	-	expression tag	UNP Q28146
B	1340	ALA	-	expression tag	UNP Q28146
B	1341	SER	-	expression tag	UNP Q28146
B	1342	THR	-	expression tag	UNP Q28146
B	1343	SER	-	expression tag	UNP Q28146
B	1344	HIS	-	expression tag	UNP Q28146
B	1345	HIS	-	expression tag	UNP Q28146
B	1346	HIS	-	expression tag	UNP Q28146
B	1347	HIS	-	expression tag	UNP Q28146
B	1348	HIS	-	expression tag	UNP Q28146
B	1349	HIS	-	expression tag	UNP Q28146

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

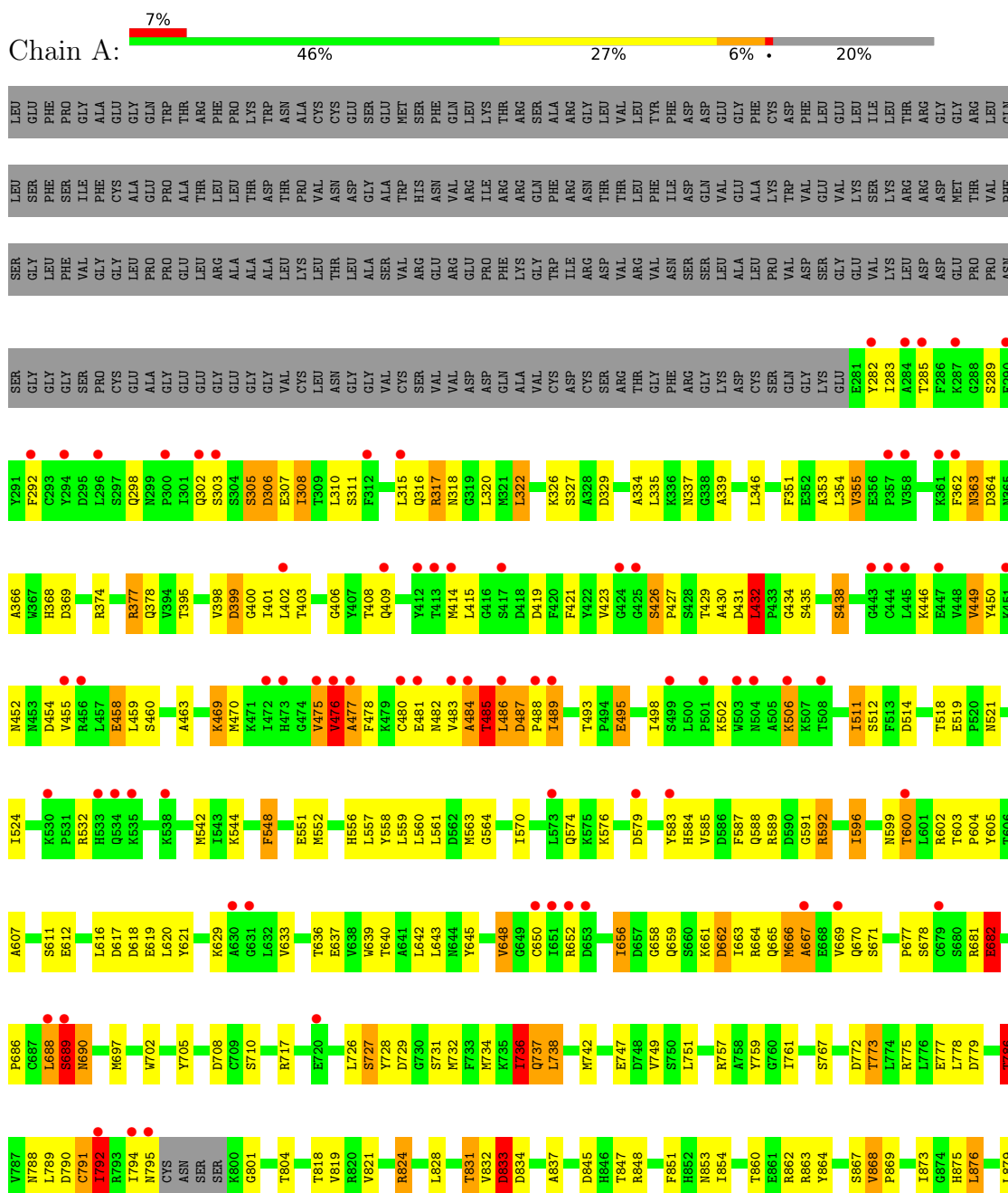


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

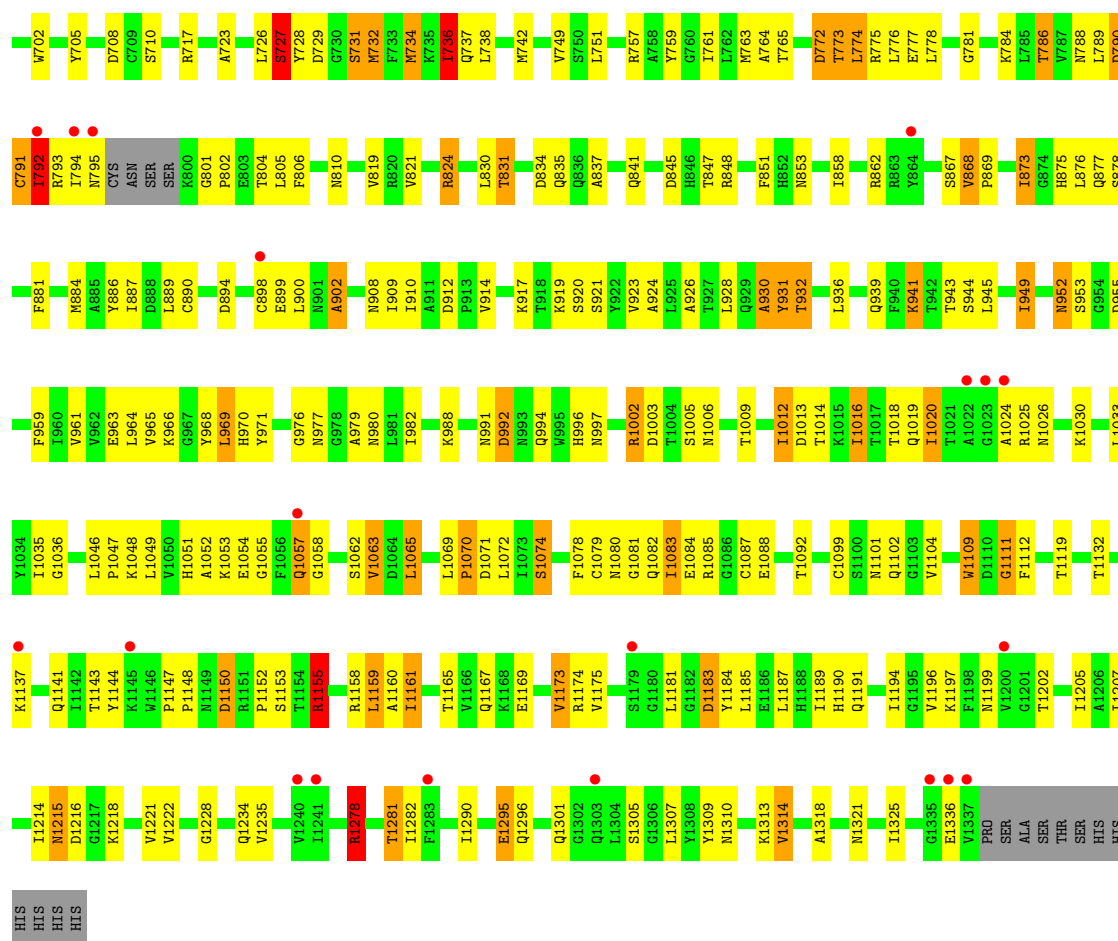
3 Residue-property plots

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: Neurexin-1-alpha







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

Chain C: 100%

MAG1
MAG2

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

Chain D: 50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.03Å 114.57Å 160.13Å 89.60° 89.98° 87.96°	Depositor
Resolution (Å)	44.29 – 2.95 44.29 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.29-2.95) 98.1 (44.29-2.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.96Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.235 0.203 , 0.231	Depositor DCC
R_{free} test set	4662 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.125 for h,-k,-l 0.004 for -h,k,-l 0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15522	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.45	54/7886 (0.7%)	1.46	88/10691 (0.8%)
1	B	1.46	68/7886 (0.9%)	1.47	85/10691 (0.8%)
All	All	1.46	122/15772 (0.8%)	1.47	173/21382 (0.8%)

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

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

All (122) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1057	GLN	CG-CD	12.54	1.83	1.52
1	B	1057	GLN	CG-CD	12.23	1.82	1.52
1	A	1036	GLY	C-O	9.14	1.36	1.24
1	A	902	ALA	CA-CB	-8.65	1.40	1.53
1	B	902	ALA	CA-CB	-8.18	1.40	1.53
1	A	909	ILE	CA-CB	-8.09	1.44	1.54
1	B	552	MET	CA-C	8.09	1.63	1.52
1	A	909	ILE	CA-C	7.87	1.61	1.52
1	A	761	ILE	C-O	7.74	1.33	1.24
1	B	1035	ILE	CA-CB	-7.53	1.45	1.54
1	B	926	ALA	CA-CB	-7.35	1.40	1.53
1	B	873	ILE	CA-CB	7.28	1.63	1.54
1	A	926	ALA	CA-CB	-7.22	1.41	1.53
1	A	1083	ILE	CA-CB	-7.19	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	912	ASP	CA-C	-7.16	1.48	1.53
1	B	1036	GLY	C-O	7.10	1.33	1.24
1	A	930	ALA	N-CA	7.08	1.55	1.46
1	A	761	ILE	CA-C	7.05	1.60	1.52
1	A	736	ILE	CA-CB	-6.99	1.46	1.54
1	B	909	ILE	CA-C	6.95	1.60	1.52
1	A	1062	SER	C-O	-6.95	1.14	1.23
1	B	1062	SER	C-O	-6.87	1.14	1.23
1	B	1282	ILE	CA-CB	-6.82	1.46	1.54
1	A	979	ALA	C-O	-6.81	1.15	1.23
1	A	690	ASN	C-O	-6.77	1.20	1.23
1	B	723	ALA	CA-CB	-6.71	1.43	1.53
1	B	764	ALA	CA-CB	-6.71	1.42	1.53
1	A	945	LEU	CA-C	-6.66	1.43	1.52
1	A	285	THR	CA-CB	6.56	1.61	1.52
1	A	1035	ILE	CA-CB	-6.54	1.46	1.54
1	B	821	VAL	CA-CB	-6.37	1.46	1.54
1	B	1035	ILE	CA-C	6.35	1.60	1.52
1	B	980	ASN	C-O	6.25	1.31	1.23
1	A	792	ILE	CA-CB	6.24	1.62	1.54
1	B	979	ALA	C-O	-6.18	1.16	1.23
1	A	596	ILE	CA-CB	6.16	1.62	1.54
1	B	997	ASN	CA-C	-6.15	1.45	1.52
1	A	1062	SER	CA-C	-6.14	1.45	1.53
1	B	945	LEU	CA-C	-6.13	1.44	1.52
1	B	917	LYS	CA-C	-6.07	1.44	1.52
1	B	1078	PHE	C-O	-6.07	1.18	1.24
1	A	910	ILE	CA-CB	-6.04	1.46	1.54
1	B	945	LEU	C-O	-6.04	1.16	1.24
1	B	761	ILE	CA-C	6.02	1.59	1.52
1	B	1083	ILE	C-O	-6.01	1.17	1.24
1	A	945	LEU	C-O	-5.98	1.16	1.24
1	B	923	VAL	CA-C	-5.96	1.45	1.52
1	A	887	ILE	CA-CB	-5.93	1.46	1.54
1	B	285	THR	CA-CB	5.89	1.60	1.52
1	A	876	LEU	N-CA	-5.87	1.38	1.45
1	A	1035	ILE	C-O	5.84	1.30	1.24
1	B	571	LYS	C-O	5.83	1.31	1.24
1	B	868	VAL	CB-CG2	-5.83	1.33	1.52
1	A	860	THR	CA-C	-5.82	1.44	1.52
1	B	732	MET	CA-C	-5.80	1.45	1.52
1	A	898	CYS	CB-SG	5.79	2.00	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1161	ILE	CA-CB	-5.79	1.49	1.55
1	B	910	ILE	CA-C	5.79	1.59	1.52
1	B	968	TYR	CA-CB	-5.78	1.44	1.53
1	A	409	GLN	CA-CB	5.78	1.61	1.53
1	B	887	ILE	CA-CB	-5.77	1.47	1.54
1	B	476	VAL	CA-CB	5.77	1.62	1.54
1	A	773	THR	CA-CB	5.76	1.63	1.53
1	A	971	TYR	CA-C	-5.75	1.45	1.52
1	A	476	VAL	CA-CB	5.74	1.62	1.54
1	B	930	ALA	N-CA	5.73	1.53	1.46
1	B	1109	TRP	CA-C	-5.72	1.45	1.52
1	B	912	ASP	C-O	-5.70	1.21	1.23
1	A	980	ASN	C-O	5.65	1.30	1.23
1	B	1002	ARG	CA-C	-5.65	1.45	1.52
1	A	1058	GLY	C-O	-5.64	1.17	1.23
1	A	834	ASP	CA-C	-5.53	1.44	1.52
1	B	792	ILE	CA-CB	5.53	1.61	1.54
1	A	968	TYR	CA-CB	-5.52	1.44	1.53
1	A	818	THR	CA-CB	-5.52	1.45	1.53
1	B	963	GLU	CD-OE2	5.52	1.35	1.25
1	A	1033	LEU	CA-C	-5.50	1.45	1.52
1	B	1016	ILE	CA-CB	5.48	1.61	1.54
1	B	1083	ILE	CA-CB	-5.46	1.47	1.54
1	B	596	ILE	CA-CB	5.41	1.61	1.54
1	B	810	ASN	CA-C	-5.41	1.45	1.53
1	B	858	ILE	C-O	-5.39	1.18	1.24
1	B	1074	SER	C-O	-5.38	1.17	1.24
1	A	879	LEU	CA-C	5.38	1.59	1.52
1	A	1057	GLN	CB-CG	5.34	1.68	1.52
1	A	964	LEU	CA-C	-5.30	1.46	1.52
1	B	1111	GLY	N-CA	5.28	1.50	1.45
1	B	409	GLN	CA-CB	5.28	1.61	1.53
1	B	943	THR	CA-CB	-5.27	1.46	1.53
1	A	1016	ILE	CG1-CD1	5.26	1.72	1.51
1	B	1016	ILE	CG1-CD1	5.25	1.72	1.51
1	B	1202	THR	CA-C	5.24	1.55	1.52
1	B	952	ASN	CA-C	5.22	1.58	1.52
1	B	890	CYS	CA-CB	-5.21	1.45	1.53
1	A	786	THR	N-CA	5.20	1.52	1.46
1	B	484	ALA	CA-C	5.20	1.59	1.52
1	B	331	VAL	CA-CB	5.18	1.61	1.54
1	B	727	SER	C-O	-5.18	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	994	GLN	CD-NE2	5.17	1.44	1.33
1	B	772	ASP	CA-C	-5.15	1.46	1.52
1	B	736	ILE	CA-CB	-5.15	1.48	1.54
1	A	1057	GLN	CD-NE2	5.14	1.44	1.33
1	A	1083	ILE	C-O	-5.14	1.18	1.24
1	B	1063	VAL	N-CA	-5.13	1.40	1.46
1	B	1020	ILE	CA-CB	-5.11	1.48	1.54
1	A	1020	ILE	CA-C	-5.10	1.46	1.52
1	B	834	ASP	CA-C	-5.10	1.45	1.52
1	B	773	THR	CA-CB	5.10	1.62	1.53
1	A	864	TYR	C-O	-5.09	1.17	1.24
1	A	943	THR	CA-CB	-5.08	1.46	1.53
1	A	919	LYS	C-O	5.08	1.29	1.24
1	B	890	CYS	N-CA	-5.08	1.40	1.46
1	B	924	ALA	CA-CB	-5.07	1.44	1.53
1	B	1161	ILE	CA-CB	-5.06	1.47	1.55
1	B	1109	TRP	C-O	-5.04	1.17	1.24
1	A	868	VAL	CB-CG2	-5.04	1.35	1.52
1	A	963	GLU	CD-OE2	5.04	1.34	1.25
1	A	767	SER	C-O	-5.04	1.18	1.24
1	B	472	ILE	CA-CB	5.04	1.60	1.53
1	B	1062	SER	CA-C	-5.04	1.46	1.53
1	A	881	PHE	CA-C	-5.02	1.47	1.52
1	B	910	ILE	CA-CB	-5.01	1.48	1.54

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1119	THR	CA-C-N	-10.32	105.52	122.65
1	A	1119	THR	C-N-CA	-10.32	105.52	122.65
1	B	1119	THR	CA-C-N	-9.07	107.59	122.65
1	B	1119	THR	C-N-CA	-9.07	107.59	122.65
1	B	426	SER	N-CA-C	8.88	115.97	108.07
1	A	432	LEU	CA-C-N	8.60	128.66	119.89
1	A	432	LEU	C-N-CA	8.60	128.66	119.89
1	B	794	ILE	N-CA-C	8.44	121.03	108.54
1	A	1046	LEU	N-CA-C	-7.91	101.03	110.13
1	A	689	SER	CA-C-N	7.90	130.69	123.10
1	A	689	SER	C-N-CA	7.90	130.69	123.10
1	B	801	GLY	CA-C-N	-7.52	112.72	120.85
1	B	801	GLY	C-N-CA	-7.52	112.72	120.85
1	B	777	GLU	N-CA-C	7.48	120.44	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	LEU	N-CA-C	7.40	120.11	108.79
1	A	1014	THR	CA-C-N	-7.38	112.59	123.00
1	A	1014	THR	C-N-CA	-7.38	112.59	123.00
1	A	637	GLU	N-CA-C	-7.36	104.10	113.23
1	B	478	PHE	N-CA-C	7.35	121.97	112.41
1	A	909	ILE	N-CA-C	7.33	118.57	108.89
1	B	1048	LYS	CA-C-N	-7.33	112.25	123.17
1	B	1048	LYS	C-N-CA	-7.33	112.25	123.17
1	A	1013	ASP	CA-C-N	-7.26	111.64	122.83
1	A	1013	ASP	C-N-CA	-7.26	111.64	122.83
1	B	705	TYR	N-CA-C	-7.21	98.97	110.14
1	A	426	SER	N-CA-C	7.12	114.41	108.07
1	B	801	GLY	N-CA-C	-7.12	97.82	112.34
1	A	801	GLY	CA-C-N	-7.06	113.22	120.85
1	A	801	GLY	C-N-CA	-7.06	113.22	120.85
1	A	794	ILE	N-CA-C	6.98	118.79	109.37
1	A	322	LEU	N-CA-C	6.92	119.38	108.79
1	A	819	VAL	CB-CA-C	-6.91	100.40	110.63
1	B	1147	PRO	CA-C-N	6.89	128.46	119.84
1	B	1147	PRO	C-N-CA	6.89	128.46	119.84
1	B	485	THR	N-CA-C	6.87	125.43	110.80
1	B	1035	ILE	N-CA-C	6.86	117.72	108.11
1	A	777	GLU	N-CA-C	6.83	119.46	109.07
1	B	1053	LYS	CD-CE-NZ	-6.83	90.05	111.90
1	A	459	LEU	N-CA-C	6.75	118.71	111.36
1	A	1147	PRO	CA-C-N	6.74	128.27	119.84
1	A	1147	PRO	C-N-CA	6.74	128.27	119.84
1	A	1074	SER	N-CA-C	6.69	120.71	112.54
1	B	992	ASP	N-CA-C	-6.69	105.88	112.97
1	B	1046	LEU	N-CA-C	-6.62	101.48	110.36
1	A	705	TYR	N-CA-C	-6.58	99.95	110.14
1	B	1111	GLY	CA-C-O	-6.57	117.58	122.37
1	A	786	THR	CA-C-N	-6.56	116.72	122.96
1	A	786	THR	C-N-CA	-6.56	116.72	122.96
1	A	1048	LYS	CA-C-N	-6.53	113.45	123.17
1	A	1048	LYS	C-N-CA	-6.53	113.45	123.17
1	B	789	LEU	N-CA-C	6.48	121.99	113.30
1	B	1070	PRO	CB-CA-C	-6.48	102.94	111.23
1	A	992	ASP	N-CA-C	-6.47	105.25	112.57
1	B	1111	GLY	N-CA-C	-6.46	105.56	112.08
1	B	1119	THR	N-CA-C	-6.43	101.87	110.55
1	B	487	ASP	CA-C-N	6.41	127.64	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	487	ASP	C-N-CA	6.41	127.64	120.66
1	B	634	PHE	CA-C-N	-6.34	113.42	119.76
1	B	634	PHE	C-N-CA	-6.34	113.42	119.76
1	A	941	LYS	CD-CE-NZ	-6.33	91.65	111.90
1	B	1012	ILE	CB-CA-C	-6.31	101.81	110.77
1	A	524	ILE	N-CA-C	6.29	116.46	110.74
1	B	667	ALA	N-CA-C	-6.27	104.79	112.88
1	B	1074	SER	N-CA-C	6.25	120.64	112.89
1	B	941	LYS	CD-CE-NZ	-6.18	92.11	111.90
1	A	791	CYS	N-CA-C	6.15	119.59	109.94
1	A	1087	CYS	CA-CB-SG	-6.12	100.33	114.40
1	B	435	SER	CA-C-N	6.06	127.41	119.84
1	B	435	SER	C-N-CA	6.06	127.41	119.84
1	B	909	ILE	N-CA-C	6.03	116.84	108.89
1	B	1081	GLY	CA-C-N	-6.02	114.56	123.11
1	B	1081	GLY	C-N-CA	-6.02	114.56	123.11
1	B	671	SER	N-CA-C	6.01	119.94	112.24
1	A	1070	PRO	CB-CA-C	-6.01	103.53	111.23
1	A	487	ASP	CA-C-N	6.01	127.34	120.85
1	A	487	ASP	C-N-CA	6.01	127.34	120.85
1	B	692	CYS	N-CA-C	6.00	117.97	108.67
1	B	976	GLY	N-CA-C	-5.99	106.70	115.63
1	A	982	ILE	CA-C-N	-5.98	113.75	122.19
1	A	982	ILE	C-N-CA	-5.98	113.75	122.19
1	A	801	GLY	N-CA-C	-5.98	100.14	112.34
1	B	774	LEU	CA-C-N	-5.97	113.31	122.62
1	B	774	LEU	C-N-CA	-5.97	113.31	122.62
1	B	819	VAL	CB-CA-C	-5.96	101.74	110.62
1	B	432	LEU	CA-C-N	5.94	126.27	119.92
1	B	432	LEU	C-N-CA	5.94	126.27	119.92
1	A	1111	GLY	N-CA-C	-5.93	105.99	112.04
1	A	1053	LYS	CD-CE-NZ	-5.93	92.92	111.90
1	A	485	THR	N-CA-C	5.92	123.41	110.80
1	B	1014	THR	CA-C-N	-5.88	114.70	123.00
1	B	1014	THR	C-N-CA	-5.88	114.70	123.00
1	B	949	ILE	CB-CA-C	-5.87	101.66	111.29
1	A	667	ALA	N-CA-C	-5.87	105.31	112.88
1	B	982	ILE	CA-C-N	-5.86	113.93	122.19
1	B	982	ILE	C-N-CA	-5.86	113.93	122.19
1	A	1111	GLY	CA-C-O	-5.82	118.26	122.45
1	A	478	PHE	N-CA-C	5.80	121.12	112.94
1	A	908	ASN	N-CA-C	-5.79	101.33	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1019	GLN	CA-C-N	-5.79	115.55	123.14
1	B	1019	GLN	C-N-CA	-5.79	115.55	123.14
1	A	854	ILE	N-CA-C	-5.78	99.32	107.75
1	A	316	GLN	N-CA-C	5.74	119.44	110.32
1	B	908	ASN	N-CA-C	-5.74	101.35	109.96
1	B	781	GLY	N-CA-C	-5.70	108.30	115.08
1	B	1167	GLN	N-CA-C	5.70	118.10	110.35
1	B	1175	VAL	CB-CA-C	-5.68	102.67	110.96
1	B	523	LEU	N-CA-C	5.66	117.30	109.15
1	A	788	ASN	CA-C-N	-5.65	113.73	122.49
1	A	788	ASN	C-N-CA	-5.65	113.73	122.49
1	B	637	GLU	N-CA-C	-5.63	105.90	112.89
1	A	1052	ALA	N-CA-C	5.60	118.47	110.24
1	A	1167	GLN	N-CA-C	5.58	117.95	110.35
1	A	671	SER	N-CA-C	5.57	119.37	112.24
1	A	821	VAL	CB-CA-C	-5.55	102.56	110.83
1	B	1099	CYS	CA-C-N	-5.54	113.85	122.37
1	B	1099	CYS	C-N-CA	-5.54	113.85	122.37
1	B	971	TYR	N-CA-C	-5.53	99.50	108.52
1	A	789	LEU	N-CA-C	5.53	120.70	113.30
1	A	738	LEU	N-CA-C	5.50	115.92	109.60
1	A	1058	GLY	CA-C-O	-5.48	116.70	122.01
1	A	1104	VAL	CB-CA-C	5.48	118.99	110.83
1	B	898	CYS	N-CA-C	-5.47	100.25	109.07
1	B	736	ILE	CA-C-N	-5.47	115.24	122.85
1	B	736	ILE	C-N-CA	-5.47	115.24	122.85
1	B	765	THR	N-CA-C	-5.47	101.25	109.95
1	B	1058	GLY	CA-C-O	-5.46	116.71	122.01
1	B	835	GLN	N-CA-C	-5.45	102.69	110.59
1	A	1175	VAL	CB-CA-C	-5.44	103.02	110.96
1	B	1109	TRP	N-CA-C	-5.43	105.52	111.82
1	B	775	ARG	N-CA-C	5.41	118.05	109.50
1	B	1155	ARG	N-CA-CB	5.40	118.47	110.53
1	A	736	ILE	CA-C-N	-5.39	115.36	122.85
1	A	736	ILE	C-N-CA	-5.39	115.36	122.85
1	A	833	ASP	CA-C-N	-5.39	114.05	122.73
1	A	833	ASP	C-N-CA	-5.39	114.05	122.73
1	B	902	ALA	N-CA-C	-5.39	103.78	110.41
1	A	981	LEU	CA-C-N	-5.38	115.94	123.10
1	A	981	LEU	C-N-CA	-5.38	115.94	123.10
1	B	484	ALA	N-CA-C	5.37	122.25	110.80
1	A	1282	ILE	N-CA-C	5.33	116.39	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1012	ILE	CB-CA-C	-5.33	103.20	110.77
1	A	920	SER	N-CA-C	5.32	122.12	110.80
1	B	977	ASN	CB-CA-C	5.27	119.29	110.44
1	A	1035	ILE	N-CA-C	5.26	115.47	108.11
1	A	1099	CYS	CA-C-N	-5.26	114.27	122.37
1	A	1099	CYS	C-N-CA	-5.26	114.27	122.37
1	B	356	GLU	N-CA-C	5.25	117.53	110.29
1	B	316	GLN	N-CA-C	5.24	118.66	110.32
1	A	971	TYR	N-CA-C	-5.23	99.88	108.41
1	A	737	GLN	CA-C-N	-5.21	112.95	120.51
1	A	737	GLN	C-N-CA	-5.21	112.95	120.51
1	B	403	THR	N-CA-C	5.21	117.44	110.35
1	A	1081	GLY	CA-C-N	-5.19	115.74	123.11
1	A	1081	GLY	C-N-CA	-5.19	115.74	123.11
1	A	863	ARG	N-CA-CB	-5.18	102.29	110.06
1	A	1119	THR	N-CA-C	-5.17	103.86	110.53
1	B	1013	ASP	CA-C-N	-5.17	114.87	122.83
1	B	1013	ASP	C-N-CA	-5.17	114.87	122.83
1	A	1134	ILE	CB-CA-C	-5.16	104.71	110.96
1	B	552	MET	CA-C-N	5.13	129.88	122.44
1	B	552	MET	C-N-CA	5.13	129.88	122.44
1	B	517	THR	N-CA-C	5.12	116.30	108.42
1	A	1149	ASN	CA-C-N	-5.11	114.96	122.83
1	A	1149	ASN	C-N-CA	-5.11	114.96	122.83
1	A	484	ALA	N-CA-C	5.08	121.62	110.80
1	A	1021	THR	N-CA-C	5.08	117.00	109.69
1	A	1049	LEU	CA-C-N	-5.06	116.42	122.90
1	A	1049	LEU	C-N-CA	-5.06	116.42	122.90
1	A	977	ASN	CB-CA-C	5.05	119.33	110.64
1	B	698	CYS	CA-CB-SG	-5.02	102.85	114.40
1	A	890	CYS	CA-CB-SG	-5.01	102.87	114.40
1	B	574	GLN	CA-C-N	5.01	128.32	120.75
1	B	574	GLN	C-N-CA	5.01	128.32	120.75

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1215	ASN	Peptide
1	A	484	ALA	Peptide
1	A	747	GLU	Peptide
1	B	1215	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	B	484	ALA	Peptide
1	B	790	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7733	0	7482	264	0
1	B	7733	0	7482	273	0
2	C	28	0	25	0	0
2	D	28	0	25	4	0
All	All	15522	0	15014	528	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 17.

All (528) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1057:GLN:CG	1:B:1057:GLN:CD	1.82	1.50
1:A:1057:GLN:CD	1:A:1057:GLN:CG	1.83	1.48
1:B:519:GLU:HG3	1:B:648:VAL:HG22	1.40	1.02
1:A:988:LYS:HG3	1:B:731:SER:HB3	1.41	1.02
1:A:727:SER:HB2	1:A:875:HIS:CD2	1.94	1.01
1:A:519:GLU:HG3	1:A:648:VAL:HG22	1.42	0.99
1:B:1278:ARG:HH11	1:B:1278:ARG:HB3	1.26	0.99
1:B:727:SER:HB2	1:B:875:HIS:CD2	1.96	0.99
1:A:1024:ALA:O	1:A:1026:ASN:ND2	1.96	0.98
1:A:1278:ARG:HB3	1:A:1278:ARG:HH11	1.24	0.97
1:B:667:ALA:HA	1:B:670:GLN:HB2	1.47	0.94
1:A:486:LEU:HG	1:A:662:ASP:HB2	1.49	0.94
1:A:599:ASN:O	1:A:600:THR:HB	1.65	0.93
1:A:618:ASP:HB3	1:A:619:GLU:OE2	1.69	0.91
1:B:1155:ARG:HG3	1:B:1155:ARG:HH11	1.37	0.89
1:A:667:ALA:HA	1:A:670:GLN:HB2	1.53	0.89
1:B:1228:GLY:HA3	1:B:1281:THR:HG22	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:751:LEU:C	1:B:751:LEU:HD12	2.00	0.86
1:A:1278:ARG:HB3	1:A:1278:ARG:NH1	1.90	0.86
1:B:1071:ASP:OD2	1:B:1074:SER:HB2	1.75	0.85
1:B:618:ASP:HB3	1:B:619:GLU:OE2	1.75	0.85
1:B:738:LEU:HD12	1:B:738:LEU:H	1.42	0.84
1:A:519:GLU:HG3	1:A:648:VAL:CG2	2.06	0.84
1:A:1183:ASP:HA	1:A:1199:ASN:O	1.79	0.82
1:A:1025:ARG:HD2	2:D:1:NAG:H83	1.62	0.82
1:A:599:ASN:O	1:A:600:THR:CB	2.28	0.81
1:B:599:ASN:O	1:B:600:THR:HB	1.82	0.80
1:B:952:ASN:HD22	1:B:953:SER:N	1.78	0.80
1:B:1155:ARG:HG3	1:B:1155:ARG:NH1	1.95	0.80
1:A:688:LEU:C	1:A:690:ASN:H	1.89	0.80
1:B:519:GLU:HG3	1:B:648:VAL:CG2	2.12	0.79
1:A:738:LEU:H	1:A:738:LEU:HD12	1.48	0.79
1:A:1101:ASN:O	1:A:1102:GLN:HB2	1.83	0.79
1:B:1278:ARG:HB3	1:B:1278:ARG:NH1	1.97	0.79
1:B:751:LEU:HD12	1:B:751:LEU:O	1.82	0.79
1:B:1174:ARG:HD3	1:B:1296:GLN:HE21	1.47	0.79
1:A:728:TYR:CE2	1:A:876:LEU:HD12	2.18	0.79
1:A:1228:GLY:HA3	1:A:1281:THR:HG22	1.65	0.78
1:B:738:LEU:HD12	1:B:738:LEU:N	1.99	0.77
1:A:988:LYS:CG	1:B:731:SER:HB3	2.14	0.77
1:B:1024:ALA:O	1:B:1026:ASN:ND2	2.17	0.77
1:B:667:ALA:HA	1:B:670:GLN:CB	2.14	0.76
1:B:431:ASP:O	1:B:432:LEU:C	2.29	0.74
1:A:305:SER:O	1:A:306:ASP:HB3	1.87	0.74
1:A:1161:ILE:HD12	1:A:1307:LEU:HB2	1.68	0.74
1:B:1101:ASN:O	1:B:1102:GLN:HB2	1.88	0.73
1:A:726:LEU:HD22	1:A:902:ALA:CB	2.18	0.73
1:A:488:PRO:HB3	1:A:652:ARG:HB3	1.71	0.73
1:A:667:ALA:HA	1:A:670:GLN:CB	2.18	0.73
1:B:426:SER:HB2	1:B:427:PRO:HD2	1.71	0.73
1:B:452:ASN:ND2	1:B:454:ASP:H	1.87	0.72
1:A:1174:ARG:HD3	1:A:1296:GLN:HE21	1.54	0.72
1:A:751:LEU:HD12	1:A:751:LEU:C	2.15	0.72
1:B:305:SER:O	1:B:306:ASP:HB3	1.88	0.72
1:B:587:PHE:CD1	1:B:587:PHE:C	2.66	0.72
1:B:353:ALA:O	1:B:354:LEU:HD12	1.90	0.72
1:A:548:PHE:O	1:A:548:PHE:CD2	2.43	0.71
1:A:738:LEU:HD12	1:A:738:LEU:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ASN:ND2	1:A:454:ASP:H	1.88	0.70
1:B:587:PHE:C	1:B:587:PHE:HD1	1.99	0.70
1:B:318:ASN:HA	1:B:335:LEU:O	1.91	0.70
1:A:688:LEU:C	1:A:690:ASN:N	2.47	0.70
1:B:688:LEU:C	1:B:690:ASN:H	1.96	0.70
1:A:430:ALA:HB2	1:A:438:SER:HB3	1.71	0.70
1:A:353:ALA:O	1:A:354:LEU:HD12	1.92	0.69
1:B:475:VAL:O	1:B:476:VAL:HB	1.93	0.69
1:A:563:MET:CE	1:A:607:ALA:HB3	2.22	0.69
1:B:686:PRO:O	1:B:689:SER:HB3	1.93	0.69
1:A:738:LEU:HD22	1:A:742:MET:HG2	1.76	0.68
1:B:1159:LEU:C	1:B:1159:LEU:HD23	2.19	0.68
1:A:952:ASN:HD22	1:A:953:SER:N	1.92	0.68
1:B:429:THR:HG22	1:B:438:SER:HA	1.75	0.68
1:A:559:LEU:HG	1:A:560:LEU:N	2.09	0.67
1:A:431:ASP:O	1:A:432:LEU:C	2.35	0.67
1:B:306:ASP:OD2	1:B:374:ARG:HD3	1.95	0.67
1:A:302:GLN:HA	1:A:415:LEU:O	1.95	0.67
1:B:302:GLN:HA	1:B:415:LEU:O	1.94	0.66
1:A:563:MET:HE2	1:A:607:ALA:HB3	1.78	0.66
1:B:292:PHE:HB2	1:B:423:VAL:HB	1.78	0.66
1:A:1155:ARG:NH1	1:A:1155:ARG:HG3	2.11	0.65
1:B:952:ASN:HD22	1:B:952:ASN:C	2.04	0.65
1:A:589:ARG:HB3	1:A:605:TYR:OH	1.96	0.65
1:A:1155:ARG:HG3	1:A:1155:ARG:HH11	1.62	0.65
1:B:488:PRO:HB3	1:B:652:ARG:HB3	1.77	0.65
1:A:292:PHE:HB2	1:A:423:VAL:HB	1.79	0.65
1:B:1184:TYR:CD1	1:B:1184:TYR:C	2.74	0.65
1:B:688:LEU:C	1:B:690:ASN:N	2.52	0.65
1:B:1174:ARG:HD3	1:B:1296:GLN:NE2	2.12	0.65
1:A:751:LEU:HD12	1:A:751:LEU:O	1.96	0.65
1:A:426:SER:HB2	1:A:427:PRO:HD2	1.79	0.65
1:A:306:ASP:OD2	1:A:374:ARG:HD3	1.98	0.64
1:A:921:SER:HA	1:A:1080:ASN:O	1.97	0.64
1:A:548:PHE:CD2	1:A:548:PHE:C	2.71	0.64
1:A:1020:ILE:HG23	1:A:1020:ILE:O	1.98	0.64
1:A:618:ASP:CB	1:A:619:GLU:OE2	2.45	0.64
1:B:589:ARG:HB3	1:B:605:TYR:OH	1.97	0.64
1:B:751:LEU:C	1:B:751:LEU:CD1	2.71	0.64
1:B:1020:ILE:HG23	1:B:1020:ILE:O	1.96	0.64
1:A:351:PHE:CE1	1:A:406:GLY:HA3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1071:ASP:OD2	1:A:1074:SER:HB2	1.98	0.64
1:A:311:SER:HB2	1:A:446:LYS:HB3	1.79	0.63
1:A:686:PRO:O	1:A:689:SER:HB3	1.98	0.63
1:A:688:LEU:O	1:A:690:ASN:N	2.32	0.63
1:B:1150:ASP:O	1:B:1152:PRO:HD3	1.98	0.63
1:A:663:ILE:C	1:A:665:GLN:H	2.06	0.63
1:A:727:SER:HB2	1:A:875:HIS:HD2	1.55	0.63
1:B:563:MET:HE2	1:B:607:ALA:HB3	1.80	0.63
1:A:429:THR:HG22	1:A:438:SER:HA	1.79	0.62
1:A:563:MET:HE2	1:A:607:ALA:CB	2.28	0.62
1:B:538:LYS:HD2	1:B:792:ILE:HD13	1.82	0.62
1:A:432:LEU:HD12	1:A:435:SER:HB2	1.82	0.62
1:A:726:LEU:HD22	1:A:902:ALA:HB1	1.81	0.62
1:B:563:MET:CE	1:B:607:ALA:HB3	2.30	0.62
1:B:1216:ASP:OD2	1:B:1218:LYS:HB2	2.00	0.62
1:B:563:MET:HE1	1:B:592:ARG:HA	1.81	0.61
1:A:1296:GLN:H	1:A:1296:GLN:CD	2.08	0.61
1:B:602:ARG:HH11	1:B:602:ARG:HB2	1.65	0.61
1:A:318:ASN:HA	1:A:335:LEU:O	2.01	0.61
1:A:969:LEU:HG	1:A:970:HIS:N	2.14	0.61
1:A:369:ASP:HB2	1:A:399:ASP:HA	1.83	0.61
1:A:1184:TYR:CD1	1:A:1184:TYR:C	2.79	0.61
1:B:311:SER:HB2	1:B:446:LYS:HB3	1.82	0.61
1:A:1025:ARG:HH11	2:D:1:NAG:H83	1.65	0.60
1:A:1183:ASP:OD2	1:A:1183:ASP:N	2.33	0.60
1:A:502:LYS:HE2	1:A:618:ASP:H	1.66	0.60
1:A:708:ASP:OD1	1:A:710:SER:OG	2.17	0.60
1:A:1159:LEU:HD23	1:A:1159:LEU:C	2.26	0.60
1:B:738:LEU:HD22	1:B:742:MET:HG2	1.84	0.60
1:B:351:PHE:CE1	1:B:406:GLY:HA3	2.37	0.60
1:A:757:ARG:HD2	1:A:873:ILE:HD12	1.84	0.59
1:B:663:ILE:C	1:B:665:GLN:H	2.09	0.59
1:B:512:SER:HA	1:B:585:VAL:O	2.02	0.59
1:B:884:MET:HB2	1:B:886:TYR:CE1	2.37	0.59
1:B:1141:GLN:HE22	1:B:1295:GLU:HG2	1.68	0.59
1:B:900:LEU:N	1:B:900:LEU:HD23	2.18	0.59
1:B:548:PHE:HA	1:B:560:LEU:O	2.03	0.58
1:B:727:SER:HB2	1:B:875:HIS:HD2	1.60	0.58
1:B:1183:ASP:HA	1:B:1199:ASN:O	2.02	0.58
1:A:1150:ASP:O	1:A:1152:PRO:HD3	2.03	0.58
1:B:346:LEU:CD2	1:B:415:LEU:HB2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:ASP:CB	1:B:619:GLU:OE2	2.51	0.58
1:B:346:LEU:HD23	1:B:415:LEU:HB2	1.85	0.58
1:B:476:VAL:O	1:B:477:ALA:HB2	2.04	0.58
1:A:514:ASP:OD1	1:A:584:HIS:HA	2.04	0.58
1:A:726:LEU:HD22	1:A:902:ALA:HB3	1.85	0.58
1:A:476:VAL:O	1:A:477:ALA:HB2	2.04	0.57
1:B:559:LEU:HG	1:B:560:LEU:N	2.20	0.57
1:B:599:ASN:O	1:B:600:THR:CB	2.51	0.57
1:A:311:SER:HB2	1:A:446:LYS:HE2	1.86	0.57
1:B:889:LEU:CD2	1:B:894:ASP:HB2	2.35	0.57
1:A:563:MET:HE1	1:A:592:ARG:HA	1.87	0.57
1:A:1025:ARG:HD2	2:D:1:NAG:C8	2.32	0.57
1:A:1112:PHE:CD1	1:A:1112:PHE:C	2.83	0.57
1:A:1174:ARG:HD3	1:A:1296:GLN:NE2	2.20	0.57
1:A:1022:ALA:HB2	1:B:1158:ARG:HD3	1.85	0.57
1:B:1161:ILE:HD12	1:B:1307:LEU:HB2	1.86	0.57
1:A:305:SER:O	1:A:306:ASP:CB	2.53	0.56
1:B:757:ARG:HD2	1:B:873:ILE:HD12	1.87	0.56
1:A:1009:THR:HG23	1:A:1018:THR:HG22	1.87	0.56
1:B:1137:LYS:HA	1:B:1301:GLN:HE21	1.70	0.56
1:A:889:LEU:CD2	1:A:894:ASP:HB2	2.35	0.56
1:B:302:GLN:O	1:B:302:GLN:HG3	2.05	0.56
1:B:305:SER:O	1:B:306:ASP:CB	2.54	0.56
1:A:548:PHE:HA	1:A:560:LEU:O	2.06	0.56
1:B:831:THR:HB	1:B:837:ALA:HA	1.87	0.56
1:A:663:ILE:C	1:A:665:GLN:N	2.64	0.55
1:B:551:GLU:OE1	1:B:640:THR:HG23	2.06	0.55
1:A:475:VAL:O	1:A:476:VAL:HB	2.07	0.55
1:A:884:MET:HB2	1:A:886:TYR:CE1	2.41	0.55
1:A:1190:HIS:ND1	1:A:1191:GLN:HG3	2.21	0.55
1:B:1005:SER:O	1:B:1006:ASN:HB2	2.07	0.55
1:A:377:ARG:CB	1:A:408:THR:OG1	2.55	0.55
1:A:302:GLN:HG3	1:A:302:GLN:O	2.06	0.55
1:B:1183:ASP:OD2	1:B:1183:ASP:N	2.40	0.55
1:A:322:LEU:HD12	1:A:421:PHE:CE1	2.43	0.54
1:A:570:ILE:CD1	1:A:605:TYR:HB3	2.37	0.54
1:A:570:ILE:HD13	1:A:605:TYR:HB3	1.88	0.54
1:B:949:ILE:HG22	1:B:949:ILE:O	2.04	0.54
1:A:1143:THR:HG23	1:A:1290:ILE:HG12	1.88	0.54
1:A:364:ASP:OD2	1:A:366:ALA:HB3	2.08	0.54
1:A:1216:ASP:OD2	1:A:1218:LYS:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:ILE:C	1:B:665:GLN:N	2.66	0.54
1:A:532:ARG:HH21	1:A:544:LYS:HB3	1.71	0.54
1:B:426:SER:CB	1:B:427:PRO:HD2	2.36	0.54
1:B:959:PHE:CD1	1:B:959:PHE:C	2.84	0.54
1:B:1112:PHE:CD1	1:B:1112:PHE:C	2.86	0.54
1:A:931:TYR:HD1	1:A:932:THR:H	1.55	0.54
1:A:1025:ARG:CD	2:D:1:NAG:H83	2.35	0.54
1:B:430:ALA:HB2	1:B:438:SER:HB3	1.88	0.54
1:A:665:GLN:HA	1:A:669:VAL:HG23	1.89	0.54
1:B:311:SER:HB2	1:B:446:LYS:HE2	1.88	0.54
1:B:969:LEU:HD23	1:B:1012:ILE:HD11	1.89	0.54
1:B:726:LEU:HD22	1:B:902:ALA:CB	2.38	0.54
1:A:791:CYS:O	1:A:792:ILE:HD12	2.08	0.54
1:A:493:THR:C	1:A:648:VAL:HG12	2.33	0.53
1:B:486:LEU:HG	1:B:662:ASP:HB2	1.91	0.53
1:B:432:LEU:HD12	1:B:435:SER:HB2	1.89	0.53
1:B:728:TYR:CE2	1:B:876:LEU:HD12	2.44	0.53
1:A:737:GLN:O	1:A:738:LEU:C	2.51	0.53
1:B:377:ARG:CB	1:B:408:THR:OG1	2.57	0.53
1:B:786:THR:HG23	1:B:804:THR:HG22	1.89	0.53
1:A:900:LEU:HD23	1:A:900:LEU:N	2.22	0.53
1:A:1159:LEU:HD23	1:A:1160:ALA:N	2.24	0.53
1:B:563:MET:HE2	1:B:607:ALA:CB	2.39	0.53
1:A:889:LEU:HD23	1:A:894:ASP:HB2	1.91	0.53
1:A:1083:ILE:N	1:A:1083:ILE:HD12	2.24	0.53
1:B:639:TRP:CZ3	1:B:824:ARG:HB3	2.44	0.53
1:B:1159:LEU:HD23	1:B:1160:ALA:N	2.22	0.53
1:A:487:ASP:HB2	1:A:664:ARG:CB	2.38	0.53
1:A:831:THR:HB	1:A:837:ALA:HA	1.90	0.53
1:B:486:LEU:HG	1:B:662:ASP:CB	2.38	0.53
1:B:315:LEU:HD13	1:B:485:THR:HG22	1.91	0.53
1:B:1296:GLN:H	1:B:1296:GLN:CD	2.17	0.53
1:A:952:ASN:HD22	1:A:952:ASN:C	2.17	0.52
1:B:1165:THR:O	1:B:1215:ASN:HA	2.09	0.52
1:A:1015:LYS:HD3	1:B:1109:TRP:CD2	2.45	0.52
1:B:322:LEU:HD12	1:B:421:PHE:CE1	2.44	0.52
1:A:1087:CYS:SG	1:A:1087:CYS:O	2.66	0.52
1:B:1143:THR:HG23	1:B:1290:ILE:HG12	1.92	0.52
1:A:751:LEU:C	1:A:751:LEU:CD1	2.81	0.52
1:B:969:LEU:CD2	1:B:1012:ILE:HD11	2.39	0.52
1:B:1159:LEU:C	1:B:1159:LEU:CD2	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ALA:HA	1:A:470:MET:HG2	1.91	0.52
1:B:726:LEU:HD22	1:B:902:ALA:HB3	1.92	0.52
1:B:931:TYR:CD1	1:B:931:TYR:N	2.77	0.52
1:A:311:SER:CB	1:A:446:LYS:HE2	2.40	0.52
1:B:1228:GLY:CA	1:B:1281:THR:HG22	2.34	0.52
1:A:512:SER:HA	1:A:585:VAL:O	2.09	0.52
1:A:587:PHE:CD1	1:A:587:PHE:C	2.83	0.52
1:A:742:MET:HG3	1:A:851:PHE:CZ	2.45	0.52
1:B:315:LEU:O	1:B:363:ASN:HB2	2.09	0.52
1:B:369:ASP:HB2	1:B:399:ASP:HA	1.92	0.52
1:B:737:GLN:O	1:B:738:LEU:C	2.51	0.52
1:A:1296:GLN:CD	1:A:1296:GLN:N	2.68	0.52
1:A:1317:MET:HE2	1:A:1322:ASP:OD1	2.10	0.52
1:B:1009:THR:HG23	1:B:1018:THR:HG22	1.92	0.51
1:A:656:ILE:HG13	1:A:661:LYS:HG3	1.92	0.51
1:B:921:SER:HA	1:B:1080:ASN:O	2.10	0.51
1:B:742:MET:HG3	1:B:851:PHE:CZ	2.46	0.51
1:A:845:ASP:OD1	1:A:845:ASP:N	2.43	0.51
1:A:948:LEU:HD12	1:A:949:ILE:H	1.76	0.51
1:A:639:TRP:CZ3	1:A:824:ARG:HB3	2.46	0.51
1:B:532:ARG:HH21	1:B:544:LYS:HB3	1.76	0.51
1:B:570:ILE:HD13	1:B:605:TYR:HB3	1.92	0.51
1:B:889:LEU:HD23	1:B:894:ASP:HB2	1.92	0.51
1:B:1190:HIS:ND1	1:B:1191:GLN:HG3	2.25	0.51
1:A:308:ILE:HD13	1:A:450:TYR:HD1	1.76	0.51
1:B:772:ASP:OD1	1:B:790:ASP:HB2	2.11	0.51
1:A:1003:ASP:OD1	1:A:1003:ASP:C	2.54	0.51
1:A:1169:GLU:OE1	1:A:1190:HIS:HA	2.11	0.51
1:A:374:ARG:HA	1:A:378:GLN:O	2.11	0.50
1:A:1020:ILE:O	1:A:1020:ILE:CG2	2.58	0.50
1:B:738:LEU:H	1:B:738:LEU:CD1	2.20	0.50
1:B:548:PHE:CD2	1:B:548:PHE:O	2.64	0.50
1:A:476:VAL:O	1:A:477:ALA:CB	2.59	0.50
1:B:519:GLU:CG	1:B:648:VAL:HG22	2.27	0.50
1:A:322:LEU:HD12	1:A:421:PHE:HE1	1.76	0.50
1:A:438:SER:O	1:A:658:GLY:HA2	2.10	0.50
1:A:775:ARG:HG3	1:A:786:THR:OG1	2.12	0.50
1:A:346:LEU:CD2	1:A:415:LEU:HB2	2.41	0.50
1:A:868:VAL:O	1:A:869:PRO:C	2.53	0.50
1:B:502:LYS:HE2	1:B:618:ASP:H	1.77	0.50
1:A:426:SER:CB	1:A:427:PRO:HD2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:ASP:O	1:B:432:LEU:O	2.29	0.50
1:B:452:ASN:HD21	1:B:454:ASP:HB2	1.77	0.50
1:B:311:SER:CB	1:B:446:LYS:HE2	2.42	0.49
1:B:1318:ALA:HA	1:B:1325:ILE:HG21	1.93	0.49
1:A:1317:MET:CE	1:A:1322:ASP:OD1	2.60	0.49
1:B:1020:ILE:O	1:B:1020:ILE:CG2	2.60	0.49
1:A:521:ASN:HB3	1:A:645:TYR:CD2	2.48	0.49
1:A:955:ASP:OD1	1:A:1030:LYS:HG3	2.12	0.49
1:B:475:VAL:O	1:B:476:VAL:CB	2.60	0.49
1:B:613:ILE:N	1:B:613:ILE:HD12	2.27	0.49
1:B:329:ASP:OD1	1:B:414:MET:O	2.31	0.49
1:B:1137:LYS:HA	1:B:1301:GLN:NE2	2.28	0.49
1:B:656:ILE:HG13	1:B:661:LYS:HG3	1.94	0.49
1:B:1222:VAL:HG13	1:B:1222:VAL:O	2.12	0.49
1:A:1186:GLU:O	1:A:1186:GLU:HG2	2.12	0.49
1:B:955:ASP:OD1	1:B:1030:LYS:HG3	2.11	0.49
1:B:729:ASP:OD1	1:B:732:MET:HG3	2.13	0.48
1:A:480:CYS:SG	1:A:481:GLU:N	2.83	0.48
1:B:665:GLN:HA	1:B:669:VAL:HG23	1.94	0.48
1:B:686:PRO:O	1:B:689:SER:CB	2.60	0.48
1:A:298:GLN:HG2	1:A:469:LYS:HE3	1.95	0.48
1:A:946:ASP:HA	1:A:964:LEU:O	2.13	0.48
1:A:1022:ALA:CB	1:B:1158:ARG:HD3	2.42	0.48
1:A:1063:VAL:HG21	1:A:1072:LEU:HD11	1.94	0.48
1:B:364:ASP:OD2	1:B:366:ALA:HB3	2.13	0.48
1:B:587:PHE:HD1	1:B:588:GLN:N	2.11	0.48
1:B:784:LYS:HG3	1:B:806:PHE:CE1	2.47	0.48
1:A:1165:THR:O	1:A:1215:ASN:HA	2.14	0.48
1:B:681:ARG:O	1:B:682:GLU:C	2.56	0.48
1:B:965:VAL:O	1:B:966:LYS:HB2	2.13	0.48
1:A:511:ILE:CG2	1:A:587:PHE:HB3	2.43	0.48
1:B:1003:ASP:C	1:B:1003:ASP:OD1	2.55	0.48
1:A:681:ARG:HG3	1:A:702:TRP:CH2	2.48	0.48
1:A:1309:TYR:O	1:A:1310:ASN:C	2.56	0.48
1:B:320:LEU:HA	1:B:334:ALA:HB2	1.95	0.48
1:A:398:VAL:C	1:A:400:GLY:H	2.21	0.48
1:A:1002:ARG:NH1	1:A:1026:ASN:OD1	2.46	0.48
1:A:1144:TYR:HA	1:A:1325:ILE:HD13	1.96	0.48
1:A:681:ARG:O	1:A:682:GLU:C	2.56	0.48
1:A:728:TYR:HE2	1:A:876:LEU:HD12	1.75	0.48
1:B:476:VAL:O	1:B:477:ALA:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:CYS:SG	1:B:481:GLU:N	2.83	0.48
1:B:919:LYS:HG2	1:B:1055:GLY:O	2.13	0.48
1:B:949:ILE:O	1:B:949:ILE:CG2	2.59	0.48
1:B:688:LEU:O	1:B:690:ASN:N	2.47	0.48
1:B:734:MET:HE1	1:B:736:ILE:CD1	2.44	0.48
1:B:1309:TYR:O	1:B:1310:ASN:C	2.57	0.48
1:B:791:CYS:O	1:B:792:ILE:HB	2.14	0.47
1:A:519:GLU:CG	1:A:648:VAL:HG22	2.30	0.47
1:A:964:LEU:HD12	1:A:964:LEU:HA	1.50	0.47
1:A:315:LEU:O	1:A:363:ASN:HB2	2.13	0.47
1:A:1015:LYS:HD3	1:B:1109:TRP:CE2	2.49	0.47
1:A:919:LYS:HG2	1:A:1055:GLY:O	2.15	0.47
1:A:1027:LEU:HD12	1:B:1155:ARG:NE	2.29	0.47
1:A:1101:ASN:O	1:A:1102:GLN:CB	2.55	0.47
1:A:311:SER:HA	1:A:368:HIS:O	2.15	0.47
1:B:1197:LYS:HA	1:B:1205:ILE:O	2.14	0.47
1:B:1207:ILE:O	1:B:1207:ILE:HG23	2.15	0.47
1:A:728:TYR:CZ	1:A:876:LEU:HD12	2.50	0.47
1:A:759:TYR:HA	1:A:778:LEU:O	2.14	0.47
1:B:317:ARG:HG3	1:B:317:ARG:HH11	1.78	0.47
1:B:845:ASP:OD1	1:B:845:ASP:N	2.42	0.47
1:A:395:THR:HG23	1:A:403:THR:HG23	1.97	0.47
1:A:602:ARG:HH11	1:A:602:ARG:HB2	1.79	0.47
1:A:965:VAL:O	1:A:966:LYS:HB2	2.15	0.47
1:A:1159:LEU:C	1:A:1159:LEU:CD2	2.86	0.47
1:A:1307:LEU:HD23	1:A:1314:VAL:HB	1.96	0.47
1:B:317:ARG:HH11	1:B:317:ARG:CG	2.28	0.47
1:B:398:VAL:C	1:B:400:GLY:H	2.23	0.47
1:B:1092:THR:O	1:B:1111:GLY:HA2	2.14	0.47
1:A:339:ALA:HB1	1:A:355:VAL:O	2.15	0.47
1:B:311:SER:HA	1:B:368:HIS:O	2.15	0.47
1:B:320:LEU:HA	1:B:334:ALA:CB	2.45	0.47
1:B:395:THR:HG23	1:B:403:THR:HG23	1.96	0.47
1:A:589:ARG:HB3	1:A:605:TYR:HH	1.80	0.47
1:A:1141:GLN:HE22	1:A:1295:GLU:HG2	1.80	0.47
1:A:1174:ARG:HG3	1:A:1186:GLU:HB2	1.96	0.47
1:B:681:ARG:HG3	1:B:702:TRP:CH2	2.49	0.47
1:B:928:LEU:HD21	1:B:936:LEU:HD21	1.97	0.47
1:B:1101:ASN:O	1:B:1102:GLN:CB	2.58	0.47
1:A:289:SER:HB3	1:A:659:GLN:OE1	2.14	0.47
1:B:988:LYS:HE3	1:B:988:LYS:HB2	1.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1155:ARG:HH11	1:B:1155:ARG:CG	2.18	0.46
1:A:551:GLU:OE1	1:A:640:THR:HG23	2.15	0.46
1:A:317:ARG:HG3	1:A:317:ARG:HH11	1.79	0.46
1:B:655:PHE:HA	1:B:659:GLN:O	2.15	0.46
1:A:452:ASN:HD21	1:A:454:ASP:HB2	1.80	0.46
1:A:992:ASP:OD2	1:A:994:GLN:NE2	2.48	0.46
1:A:1072:LEU:HA	1:A:1072:LEU:HD23	1.53	0.46
1:B:282:TYR:HB3	1:B:460:SER:HB3	1.96	0.46
1:B:469:LYS:HD3	1:B:469:LYS:HA	1.78	0.46
1:B:969:LEU:HG	1:B:970:HIS:N	2.30	0.46
1:B:1296:GLN:CD	1:B:1296:GLN:N	2.73	0.46
1:A:779:ASP:C	1:A:779:ASP:OD1	2.59	0.46
1:A:939:GLN:HA	1:A:996:HIS:O	2.15	0.46
1:B:339:ALA:HB1	1:B:355:VAL:O	2.15	0.46
1:B:570:ILE:CD1	1:B:605:TYR:HB3	2.46	0.46
1:B:666:MET:HE2	1:B:666:MET:HB2	1.81	0.46
1:B:1072:LEU:HD23	1:B:1072:LEU:HA	1.42	0.46
1:A:556:HIS:NE2	1:A:576:LYS:HG2	2.31	0.46
1:B:1016:ILE:HG22	1:B:1018:THR:HG23	1.98	0.46
1:A:398:VAL:C	1:A:400:GLY:N	2.73	0.46
1:A:991:ASN:OD1	1:A:991:ASN:N	2.41	0.46
1:B:1002:ARG:NH1	1:B:1026:ASN:OD1	2.49	0.46
1:B:367:TRP:CZ3	1:B:446:LYS:HB2	2.52	0.45
1:A:282:TYR:HB3	1:A:460:SER:HB3	1.97	0.45
1:A:666:MET:HB2	1:A:666:MET:HE2	1.83	0.45
1:A:1214:ILE:C	1:A:1214:ILE:HD12	2.41	0.45
1:B:514:ASP:OD1	1:B:584:HIS:HA	2.16	0.45
1:B:759:TYR:HA	1:B:778:LEU:O	2.16	0.45
1:B:841:GLN:HA	1:B:841:GLN:OE1	2.16	0.45
1:B:1065:LEU:CD1	1:B:1070:PRO:HG3	2.46	0.45
1:B:772:ASP:HA	1:B:788:ASN:O	2.17	0.45
1:B:788:ASN:HD22	1:B:802:PRO:HB3	1.82	0.45
1:B:1030:LYS:HA	1:B:1030:LYS:HD3	1.82	0.45
1:A:315:LEU:HD13	1:A:485:THR:HG23	1.98	0.45
1:A:729:ASP:OD1	1:A:732:MET:HG3	2.17	0.45
1:B:586:ASP:OD2	1:B:588:GLN:NE2	2.50	0.45
1:B:332:ASN:ND2	1:B:435:SER:HA	2.32	0.45
1:B:931:TYR:HD1	1:B:932:THR:H	1.64	0.45
1:A:1024:ALA:O	1:A:1025:ARG:C	2.59	0.45
1:B:763:MET:HE1	1:B:774:LEU:HD23	1.98	0.45
1:B:322:LEU:HD12	1:B:421:PHE:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:PHE:C	1:B:364:ASP:H	2.24	0.45
1:B:685:LYS:HB2	1:B:685:LYS:HE3	1.88	0.45
1:B:952:ASN:HB2	1:B:1033:LEU:HD12	1.97	0.45
1:A:621:TYR:OH	1:A:629:LYS:HD3	2.16	0.45
1:A:786:THR:HG23	1:A:804:THR:HG22	1.98	0.45
1:B:552:MET:HA	1:B:556:HIS:O	2.16	0.45
1:B:991:ASN:OD1	1:B:991:ASN:N	2.43	0.45
1:A:377:ARG:HB3	1:A:408:THR:OG1	2.16	0.44
1:A:317:ARG:HH11	1:A:317:ARG:CG	2.30	0.44
1:B:374:ARG:HA	1:B:378:GLN:O	2.17	0.44
1:A:636:THR:HG21	1:A:848:ARG:HG3	1.98	0.44
1:A:1005:SER:O	1:A:1006:ASN:HB2	2.17	0.44
1:B:343:VAL:HG21	1:B:434:GLY:O	2.18	0.44
1:B:928:LEU:HD13	1:B:1065:LEU:HB3	1.99	0.44
1:A:362:PHE:C	1:A:364:ASP:H	2.25	0.44
1:A:999:MET:HE3	1:A:1011:LYS:HB2	2.00	0.44
1:B:308:ILE:HD13	1:B:450:TYR:HD1	1.82	0.44
1:A:959:PHE:CD1	1:A:959:PHE:C	2.94	0.44
1:A:1158:ARG:HH11	1:A:1158:ARG:HD2	1.55	0.44
1:A:736:ILE:HG12	1:A:886:TYR:CD2	2.52	0.44
1:A:1185:LEU:HD12	1:A:1186:GLU:N	2.32	0.44
1:A:579:ASP:OD2	1:A:583:TYR:OH	2.36	0.44
1:A:749:VAL:HG22	1:A:881:PHE:CD1	2.53	0.44
1:B:708:ASP:OD1	1:B:710:SER:OG	2.27	0.44
1:B:805:LEU:HD23	1:B:805:LEU:HA	1.79	0.44
1:A:931:TYR:CD1	1:A:931:TYR:N	2.84	0.44
1:A:1322:ASP:OD2	1:A:1322:ASP:C	2.61	0.44
1:B:734:MET:CE	1:B:736:ILE:CD1	2.96	0.44
1:A:489:ILE:CD1	1:A:664:ARG:HA	2.48	0.43
1:A:551:GLU:HG2	1:A:560:LEU:HD13	2.00	0.43
1:A:884:MET:CB	1:A:886:TYR:CE1	3.01	0.43
1:B:1051:HIS:O	1:B:1052:ALA:C	2.60	0.43
1:B:1132:THR:HG23	1:B:1305:SER:HB2	2.00	0.43
1:B:1158:ARG:HH11	1:B:1158:ARG:HD2	1.54	0.43
1:B:1169:GLU:HA	1:B:1189:ILE:O	2.18	0.43
1:A:1320:GLU:C	1:A:1321:ASN:HD22	2.26	0.43
1:B:636:THR:HG21	1:B:848:ARG:HG3	1.98	0.43
1:B:889:LEU:HD23	1:B:889:LEU:HA	1.53	0.43
1:B:1173:VAL:HG13	1:B:1187:LEU:HB3	2.01	0.43
1:A:1016:ILE:HG22	1:A:1018:THR:HG23	2.00	0.43
1:B:298:GLN:HG2	1:B:469:LYS:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:PRO:HD2	1:B:437:VAL:H	1.83	0.43
1:B:881:PHE:C	1:B:881:PHE:CD2	2.96	0.43
1:A:548:PHE:HD1	1:A:587:PHE:HE2	1.64	0.43
1:B:727:SER:HB2	1:B:875:HIS:NE2	2.32	0.43
1:A:310:LEU:HD12	1:A:310:LEU:O	2.19	0.43
1:A:329:ASP:OD1	1:A:414:MET:O	2.37	0.43
1:B:398:VAL:C	1:B:400:GLY:N	2.76	0.43
1:B:1144:TYR:HA	1:B:1325:ILE:HD13	2.01	0.43
1:B:663:ILE:HA	1:B:666:MET:HB2	2.01	0.43
1:A:729:ASP:CG	1:A:732:MET:HE3	2.44	0.43
1:A:1092:THR:O	1:A:1111:GLY:HA2	2.19	0.43
1:A:1134:ILE:HD12	1:A:1332:ARG:HH22	1.83	0.43
1:B:522:GLY:HA2	1:B:645:TYR:O	2.19	0.43
1:B:734:MET:CE	1:B:736:ILE:HD12	2.49	0.43
1:A:557:LEU:HG	1:A:558:TYR:N	2.33	0.43
1:A:772:ASP:OD1	1:A:790:ASP:HB2	2.19	0.43
1:A:1012:ILE:HG23	1:A:1012:ILE:HD12	1.69	0.43
1:B:708:ASP:OD1	1:B:708:ASP:C	2.62	0.43
1:B:511:ILE:HG23	1:B:587:PHE:HB3	2.01	0.42
1:B:573:LEU:HD12	1:B:574:GLN:H	1.84	0.42
1:B:1063:VAL:HG21	1:B:1072:LEU:HD11	2.01	0.42
1:B:1307:LEU:HD23	1:B:1314:VAL:HB	2.01	0.42
1:A:1071:ASP:O	1:A:1072:LEU:C	2.60	0.42
1:B:952:ASN:HD22	1:B:953:SER:H	1.62	0.42
1:A:320:LEU:HA	1:A:334:ALA:CB	2.48	0.42
1:A:488:PRO:CB	1:A:652:ARG:HB3	2.46	0.42
1:A:570:ILE:CD1	1:A:605:TYR:CB	2.97	0.42
1:A:881:PHE:C	1:A:881:PHE:CD2	2.97	0.42
1:A:988:LYS:CD	1:B:731:SER:HB3	2.49	0.42
1:B:548:PHE:CD2	1:B:548:PHE:C	2.92	0.42
1:B:521:ASN:HB3	1:B:645:TYR:CD2	2.55	0.42
1:B:532:ARG:NH2	1:B:544:LYS:HB3	2.34	0.42
1:B:793:ARG:HE	1:B:793:ARG:HB2	1.70	0.42
1:B:557:LEU:HG	1:B:558:TYR:N	2.33	0.42
1:B:294:TYR:HD2	1:B:296:LEU:HD23	1.85	0.42
1:B:523:LEU:HD11	1:B:526:PHE:HB2	2.02	0.42
1:B:952:ASN:HB2	1:B:1033:LEU:CD1	2.50	0.42
1:A:320:LEU:HA	1:A:334:ALA:HB2	2.00	0.42
1:A:1041:GLU:HA	1:A:1041:GLU:OE1	2.19	0.42
1:B:327:SER:HB2	1:B:328:ALA:H	1.46	0.42
1:A:495:GLU:OE2	1:A:495:GLU:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:GLU:HG2	1:B:560:LEU:HD13	2.01	0.41
1:B:749:VAL:HG22	1:B:881:PHE:CD1	2.55	0.41
1:B:1196:VAL:HG12	1:B:1197:LYS:N	2.35	0.41
1:A:308:ILE:CD1	1:A:450:TYR:HD1	2.33	0.41
1:B:493:THR:C	1:B:648:VAL:HG12	2.46	0.41
1:B:603:THR:HA	1:B:604:PRO:HD2	1.90	0.41
1:B:964:LEU:HD12	1:B:964:LEU:HA	1.61	0.41
1:A:832:VAL:O	1:A:833:ASP:HB2	2.19	0.41
1:B:900:LEU:HD23	1:B:900:LEU:H	1.83	0.41
1:A:449:VAL:HG13	1:A:458:GLU:HA	2.02	0.41
1:A:486:LEU:HG	1:A:662:ASP:CB	2.35	0.41
1:B:488:PRO:HB3	1:B:652:ARG:CB	2.46	0.41
1:B:1214:ILE:HD12	1:B:1214:ILE:C	2.45	0.41
1:A:791:CYS:O	1:A:792:ILE:HB	2.19	0.41
1:B:322:LEU:CD2	1:B:333:LEU:HD23	2.50	0.41
1:B:421:PHE:CD1	1:B:421:PHE:C	2.98	0.41
1:B:1087:CYS:O	1:B:1087:CYS:SG	2.79	0.41
1:A:310:LEU:HD12	1:A:310:LEU:C	2.46	0.41
1:A:488:PRO:HB3	1:A:652:ARG:CB	2.47	0.41
1:A:493:THR:HB	1:A:495:GLU:OE2	2.20	0.41
1:B:992:ASP:OD2	1:B:994:GLN:NE2	2.54	0.41
1:B:1069:LEU:HA	1:B:1070:PRO:HD2	1.91	0.41
1:A:1169:GLU:HA	1:A:1189:ILE:O	2.20	0.41
1:A:1233:LEU:HD12	1:A:1233:LEU:HA	1.65	0.41
1:B:421:PHE:C	1:B:421:PHE:HD1	2.29	0.41
1:B:1024:ALA:O	1:B:1025:ARG:C	2.63	0.41
1:A:532:ARG:NH1	1:A:564:GLY:HA2	2.36	0.41
1:A:570:ILE:HD11	1:A:605:TYR:HB2	2.03	0.41
1:A:591:GLY:HA2	1:A:612:GLU:O	2.20	0.41
1:A:738:LEU:H	1:A:738:LEU:CD1	2.27	0.41
1:B:790:ASP:OD2	1:B:791:CYS:N	2.44	0.41
1:A:495:GLU:H	1:A:495:GLU:CD	2.29	0.41
1:A:1228:GLY:CA	1:A:1281:THR:HG22	2.43	0.41
1:B:569:LYS:C	1:B:570:ILE:HG13	2.45	0.41
1:A:643:LEU:HD21	1:A:824:ARG:NH2	2.36	0.40
1:A:1027:LEU:HD12	1:B:1155:ARG:CZ	2.50	0.40
1:B:868:VAL:HB	1:B:869:PRO:HD2	2.02	0.40
1:B:1313:LYS:O	1:B:1314:VAL:C	2.64	0.40
1:A:548:PHE:CD1	1:A:587:PHE:HE2	2.39	0.40
1:A:603:THR:HA	1:A:604:PRO:HD2	1.94	0.40
1:A:896:ASP:OD1	1:A:896:ASP:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:LEU:HA	1:B:776:LEU:HD23	1.90	0.40
1:A:489:ILE:O	1:A:650:CYS:HA	2.21	0.40
1:A:512:SER:HB2	1:A:584:HIS:HE1	1.87	0.40
1:A:552:MET:HA	1:A:556:HIS:O	2.21	0.40
1:B:450:TYR:CZ	1:B:452:ASN:HB3	2.55	0.40
1:B:877:GLN:O	1:B:878:SER:HB2	2.21	0.40
1:B:939:GLN:HA	1:B:996:HIS:O	2.21	0.40
1:A:475:VAL:O	1:A:476:VAL:CB	2.70	0.40
1:A:728:TYR:CE2	1:A:876:LEU:CD1	2.99	0.40
1:A:1234:GLN:NE2	1:A:1236:ASP:O	2.55	0.40
1:A:1318:ALA:HA	1:A:1325:ILE:HG21	2.03	0.40
1:B:317:ARG:HG2	1:B:337:ASN:HA	2.03	0.40
1:B:431:ASP:C	1:B:432:LEU:O	2.61	0.40
1:B:1083:ILE:HD12	1:B:1083:ILE:N	2.36	0.40
1:A:686:PRO:O	1:A:689:SER:CB	2.69	0.40
1:A:1106:LEU:HD11	1:A:1115:ASP:HB2	2.04	0.40
1:A:1300:PHE:CG	1:A:1301:GLN:N	2.89	0.40
1:B:493:THR:HB	1:B:495:GLU:OE2	2.22	0.40
1:B:742:MET:HB3	1:B:851:PHE:CE2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	1004/1254 (80%)	881 (88%)	97 (10%)	26 (3%)	4	12
1	B	1004/1254 (80%)	881 (88%)	96 (10%)	27 (3%)	4	11
All	All	2008/2508 (80%)	1762 (88%)	193 (10%)	53 (3%)	4	12

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	SER
1	A	401	ILE
1	A	476	VAL
1	A	477	ALA
1	A	506	LYS
1	A	666	MET
1	A	677	PRO
1	A	689	SER
1	A	792	ILE
1	B	327	SER
1	B	401	ILE
1	B	476	VAL
1	B	477	ALA
1	B	506	LYS
1	B	666	MET
1	B	677	PRO
1	B	689	SER
1	B	792	ILE
1	B	1278	ARG
1	A	306	ASP
1	A	475	VAL
1	A	600	THR
1	A	682	GLU
1	A	920	SER
1	A	930	ALA
1	A	1278	ARG
1	B	434	GLY
1	B	475	VAL
1	B	682	GLU
1	B	930	ALA
1	A	399	ASP
1	A	434	GLY
1	B	399	ASP
1	B	485	THR
1	B	600	THR
1	B	664	ARG
1	B	920	SER
1	A	363	ASN
1	A	833	ASP
1	A	1045	SER
1	B	337	ASN
1	B	573	LEU
1	A	337	ASN

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Mol	Chain	Res	Type
1	A	1179	SER
1	A	1209	GLU
1	B	363	ASN
1	B	791	CYS
1	A	1148	PRO
1	B	436	PRO
1	B	1047	PRO
1	B	483	VAL
1	A	483	VAL
1	B	1148	PRO

5.3.2 Protein sidechains [i](#)

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	839/1068 (79%)	738 (88%)	101 (12%)	5	14
1	B	839/1068 (79%)	738 (88%)	101 (12%)	5	14
All	All	1678/2136 (79%)	1476 (88%)	202 (12%)	5	14

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	283	ILE
1	A	303	SER
1	A	305	SER
1	A	307	GLU
1	A	308	ILE
1	A	317	ARG
1	A	326	LYS
1	A	355	VAL
1	A	377	ARG
1	A	402	LEU
1	A	419	ASP
1	A	432	LEU
1	A	438	SER

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Mol	Chain	Res	Type
1	A	449	VAL
1	A	455	VAL
1	A	458	GLU
1	A	469	LYS
1	A	482	ASN
1	A	485	THR
1	A	486	LEU
1	A	489	ILE
1	A	495	GLU
1	A	498	ILE
1	A	506	LYS
1	A	511	ILE
1	A	518	THR
1	A	542	MET
1	A	548	PHE
1	A	561	LEU
1	A	574	GLN
1	A	588	GLN
1	A	592	ARG
1	A	596	ILE
1	A	611	SER
1	A	616	LEU
1	A	617	ASP
1	A	620	LEU
1	A	633	VAL
1	A	642	LEU
1	A	648	VAL
1	A	656	ILE
1	A	662	ASP
1	A	678	SER
1	A	682	GLU
1	A	688	LEU
1	A	697	MET
1	A	717	ARG
1	A	727	SER
1	A	731	SER
1	A	734	MET
1	A	736	ILE
1	A	773	THR
1	A	786	THR
1	A	792	ILE
1	A	795	ASN

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Mol	Chain	Res	Type
1	A	824	ARG
1	A	828	LEU
1	A	831	THR
1	A	847	THR
1	A	853	ASN
1	A	862	ARG
1	A	867	SER
1	A	898	CYS
1	A	899	GLU
1	A	914	VAL
1	A	931	TYR
1	A	932	THR
1	A	941	LYS
1	A	944	SER
1	A	969	LEU
1	A	985	SER
1	A	989	PRO
1	A	1049	LEU
1	A	1054	GLU
1	A	1068	ARG
1	A	1074	SER
1	A	1079	CYS
1	A	1082	GLN
1	A	1085	ARG
1	A	1088	GLU
1	A	1091	SER
1	A	1104	VAL
1	A	1150	ASP
1	A	1153	SER
1	A	1155	ARG
1	A	1159	LEU
1	A	1171	VAL
1	A	1173	VAL
1	A	1181	LEU
1	A	1183	ASP
1	A	1185	LEU
1	A	1221	VAL
1	A	1234	GLN
1	A	1235	VAL
1	A	1278	ARG
1	A	1281	THR
1	A	1294	LYS

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Mol	Chain	Res	Type
1	A	1295	GLU
1	A	1314	VAL
1	A	1321	ASN
1	A	1336	GLU
1	B	283	ILE
1	B	303	SER
1	B	305	SER
1	B	307	GLU
1	B	308	ILE
1	B	317	ARG
1	B	326	LYS
1	B	344	ILE
1	B	355	VAL
1	B	377	ARG
1	B	378	GLN
1	B	402	LEU
1	B	419	ASP
1	B	432	LEU
1	B	438	SER
1	B	449	VAL
1	B	455	VAL
1	B	458	GLU
1	B	482	ASN
1	B	485	THR
1	B	486	LEU
1	B	489	ILE
1	B	495	GLU
1	B	498	ILE
1	B	506	LYS
1	B	511	ILE
1	B	518	THR
1	B	542	MET
1	B	548	PHE
1	B	561	LEU
1	B	574	GLN
1	B	587	PHE
1	B	588	GLN
1	B	589	ARG
1	B	592	ARG
1	B	596	ILE
1	B	611	SER
1	B	616	LEU

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Mol	Chain	Res	Type
1	B	617	ASP
1	B	620	LEU
1	B	633	VAL
1	B	642	LEU
1	B	648	VAL
1	B	656	ILE
1	B	662	ASP
1	B	663	ILE
1	B	665	GLN
1	B	678	SER
1	B	682	GLU
1	B	688	LEU
1	B	697	MET
1	B	717	ARG
1	B	727	SER
1	B	731	SER
1	B	734	MET
1	B	736	ILE
1	B	773	THR
1	B	786	THR
1	B	795	ASN
1	B	824	ARG
1	B	830	LEU
1	B	831	THR
1	B	847	THR
1	B	853	ASN
1	B	862	ARG
1	B	867	SER
1	B	899	GLU
1	B	914	VAL
1	B	931	TYR
1	B	932	THR
1	B	941	LYS
1	B	944	SER
1	B	961	VAL
1	B	969	LEU
1	B	1049	LEU
1	B	1054	GLU
1	B	1065	LEU
1	B	1079	CYS
1	B	1082	GLN
1	B	1084	GLU

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Mol	Chain	Res	Type
1	B	1085	ARG
1	B	1088	GLU
1	B	1104	VAL
1	B	1150	ASP
1	B	1153	SER
1	B	1155	ARG
1	B	1159	LEU
1	B	1173	VAL
1	B	1181	LEU
1	B	1183	ASP
1	B	1185	LEU
1	B	1194	ILE
1	B	1221	VAL
1	B	1234	GLN
1	B	1235	VAL
1	B	1278	ARG
1	B	1281	THR
1	B	1295	GLU
1	B	1314	VAL
1	B	1321	ASN
1	B	1336	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	GLN
1	A	365	ASN
1	A	452	ASN
1	A	541	GLN
1	A	743	HIS
1	A	788	ASN
1	A	846	HIS
1	A	892	ASN
1	A	952	ASN
1	A	994	GLN
1	A	1301	GLN
1	A	1321	ASN
1	B	337	ASN
1	B	365	ASN
1	B	440	ASN
1	B	452	ASN
1	B	541	GLN

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Mol	Chain	Res	Type
1	B	588	GLN
1	B	743	HIS
1	B	788	ASN
1	B	810	ASN
1	B	846	HIS
1	B	892	ASN
1	B	952	ASN
1	B	994	GLN
1	B	1008	HIS
1	B	1141	GLN
1	B	1301	GLN
1	B	1321	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

4 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	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.89	0	17,19,21	2.94	10 (58%)
2	NAG	C	2	2	14,14,15	0.62	0	17,19,21	1.58	3 (17%)
2	NAG	D	1	1,2	14,14,15	0.84	0	17,19,21	3.03	9 (52%)
2	NAG	D	2	2	14,14,15	0.85	1 (7%)	17,19,21	1.45	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C1-C2	2.26	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	7.08	121.67	112.19
2	C	1	NAG	C1-O5-C5	6.12	120.39	112.19
2	D	1	NAG	C1-C2-N2	4.46	117.45	110.43
2	C	1	NAG	O7-C7-C8	-4.42	114.19	122.05
2	D	1	NAG	C2-N2-C7	4.37	128.76	122.90
2	C	1	NAG	C1-C2-N2	4.30	117.21	110.43
2	D	1	NAG	O7-C7-C8	-3.72	115.43	122.05
2	C	1	NAG	C2-N2-C7	3.61	127.73	122.90
2	C	1	NAG	O5-C5-C6	3.49	114.46	107.66
2	C	2	NAG	O5-C5-C6	3.41	114.30	107.66
2	D	1	NAG	O5-C5-C6	3.38	114.24	107.66
2	D	2	NAG	O5-C5-C6	3.32	114.12	107.66
2	D	1	NAG	O7-C7-N2	3.31	127.83	121.98
2	D	1	NAG	O4-C4-C3	-2.97	103.38	110.38
2	C	1	NAG	O7-C7-N2	2.92	127.14	121.98
2	C	1	NAG	C4-C3-C2	2.88	115.24	111.02
2	C	1	NAG	O4-C4-C3	-2.86	103.63	110.38
2	C	2	NAG	C1-O5-C5	-2.78	108.45	112.19
2	D	1	NAG	O6-C6-C5	2.61	120.21	111.33
2	C	2	NAG	C2-N2-C7	-2.53	119.51	122.90
2	C	1	NAG	C6-C5-C4	2.48	119.12	113.02
2	D	2	NAG	C1-O5-C5	-2.38	108.99	112.19
2	D	2	NAG	C4-C3-C2	2.35	114.46	111.02
2	C	1	NAG	O6-C6-C5	2.29	119.12	111.33
2	D	2	NAG	C2-N2-C7	-2.17	119.99	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C6-C5-C4	2.01	117.96	113.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

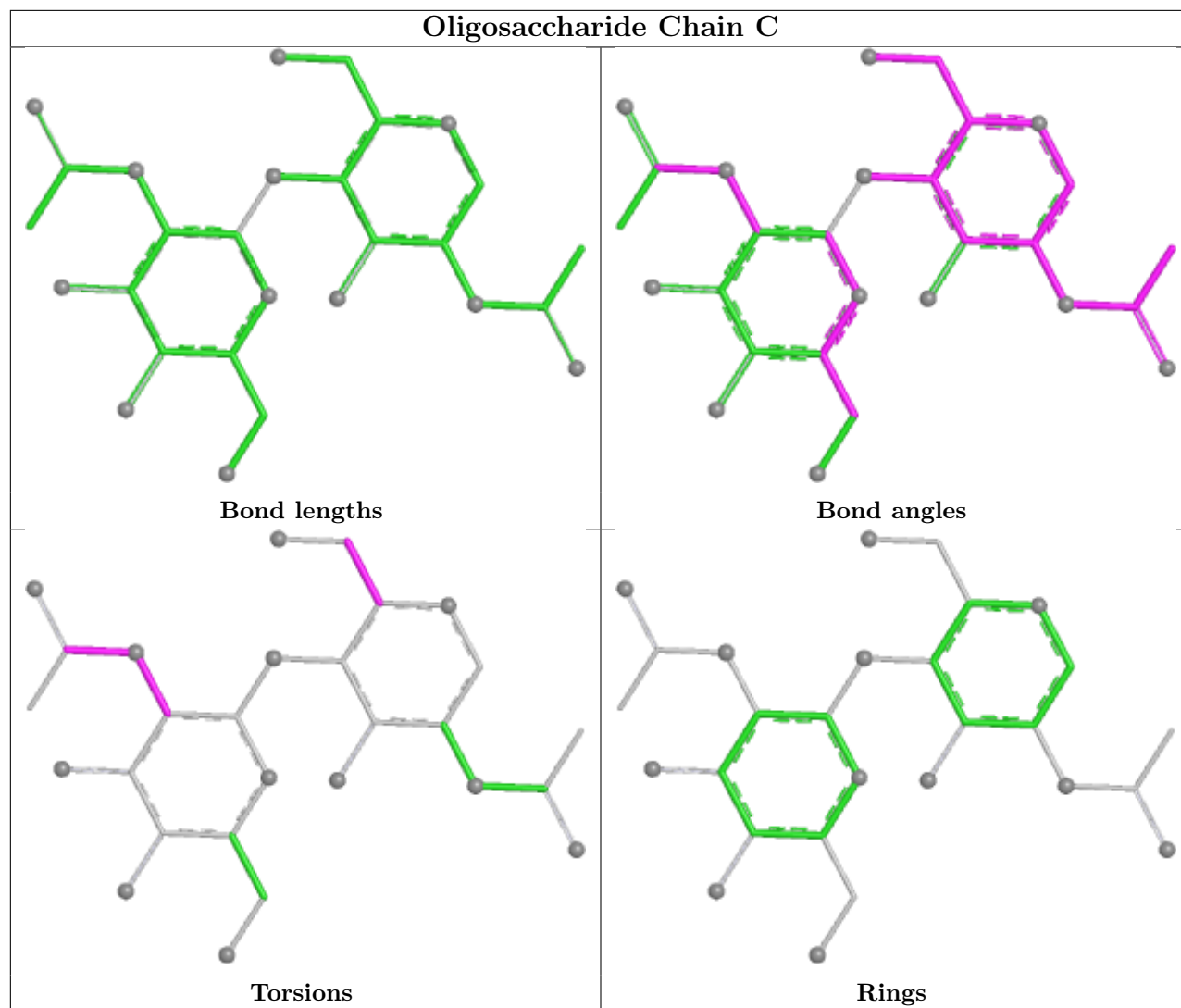
Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C8-C7-N2-C2
2	C	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C1-C2-N2-C7
2	D	2	NAG	C1-C2-N2-C7
2	D	1	NAG	O5-C5-C6-O6

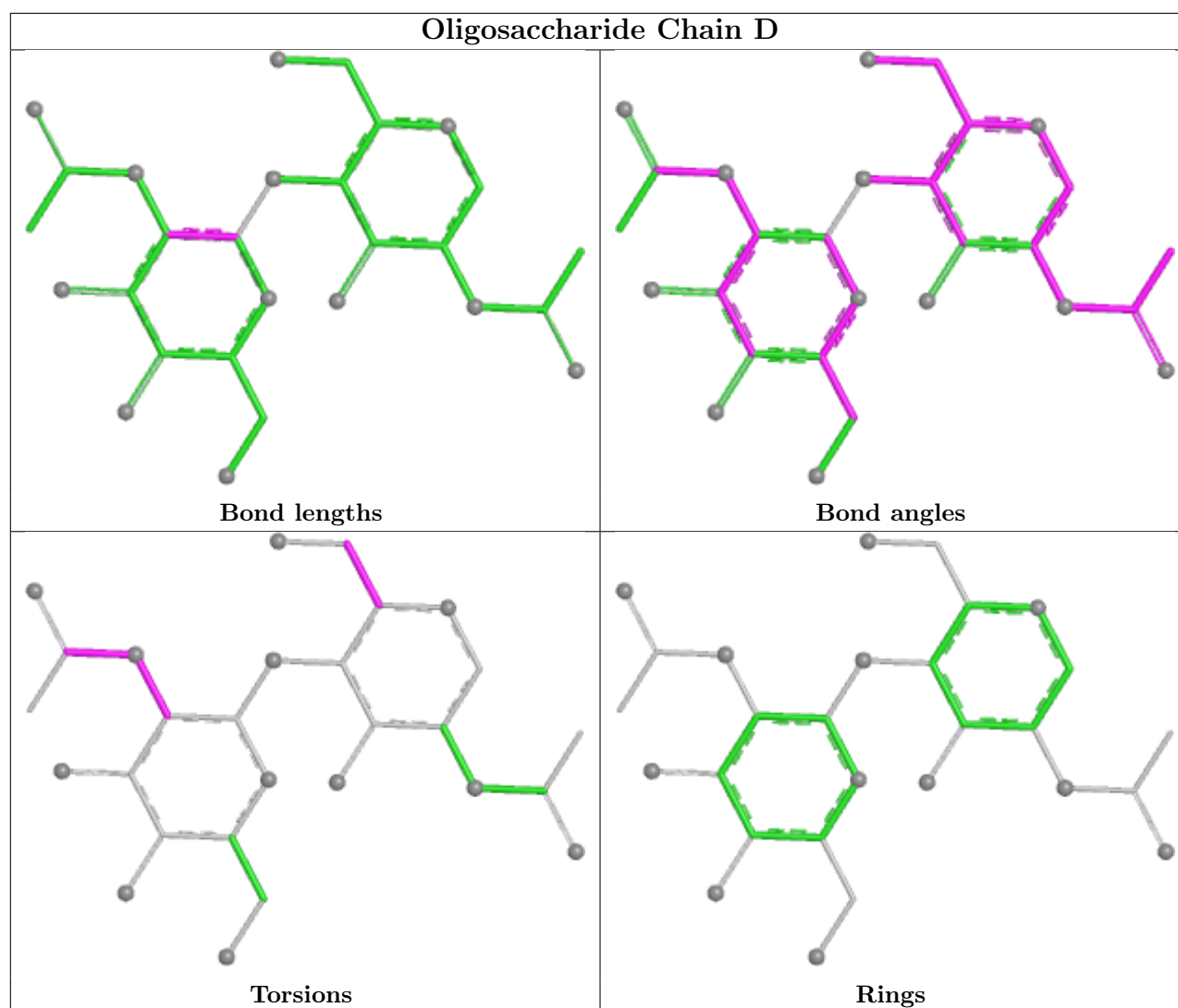
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	4	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	1008/1254 (80%)	0.40	86 (8%) 16 15	35, 91, 151, 196	0
1	B	1008/1254 (80%)	0.39	70 (6%) 23 19	34, 92, 152, 201	0
All	All	2016/2508 (80%)	0.40	156 (7%) 19 17	34, 91, 152, 201	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1337	VAL	6.7
1	A	476	VAL	6.7
1	B	476	VAL	5.7
1	B	483	VAL	5.5
1	A	484	ALA	5.4
1	B	688	LEU	5.4
1	A	1337	VAL	5.4
1	A	475	VAL	5.3
1	B	290	GLU	5.2
1	A	302	GLN	5.1
1	A	472	ILE	5.1
1	A	483	VAL	5.0
1	A	300	PRO	5.0
1	B	472	ILE	4.9
1	B	475	VAL	4.8
1	B	667	ALA	4.8
1	B	484	ALA	4.6
1	A	792	ILE	4.5
1	A	688	LEU	4.2
1	B	1023	GLY	4.2
1	A	451	LYS	4.1
1	A	445	LEU	4.1
1	B	287	LYS	4.1
1	B	1335	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	794	ILE	4.0
1	B	413	THR	4.0
1	B	402	LEU	3.9
1	A	667	ALA	3.8
1	B	414	MET	3.8
1	A	414	MET	3.7
1	A	290	GLU	3.6
1	A	652	ARG	3.5
1	B	534	GLN	3.4
1	B	1022	ALA	3.4
1	A	480	CYS	3.3
1	B	451	LYS	3.3
1	B	477	ALA	3.3
1	A	402	LEU	3.3
1	A	630	ALA	3.3
1	B	669	VAL	3.3
1	A	444	CYS	3.3
1	B	302	GLN	3.2
1	A	534	GLN	3.2
1	A	1200	VAL	3.1
1	A	1336	GLU	3.1
1	A	508	THR	3.1
1	A	287	LYS	3.0
1	A	424	GLY	3.0
1	B	600	THR	3.0
1	B	1303	GLN	3.0
1	A	898	CYS	3.0
1	A	538	LYS	2.9
1	A	583	TYR	2.9
1	B	898	CYS	2.9
1	A	651	ILE	2.9
1	A	1335	GLY	2.9
1	A	447	GLU	2.9
1	B	1336	GLU	2.9
1	A	417	SER	2.9
1	B	1024	ALA	2.9
1	B	1200	VAL	2.9
1	A	303	SER	2.9
1	A	689	SER	2.8
1	B	689	SER	2.8
1	A	425	GLY	2.8
1	A	795	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	506	LYS	2.8
1	B	616	LEU	2.8
1	A	477	ALA	2.7
1	A	499	SER	2.7
1	B	504	ASN	2.7
1	A	481	GLU	2.7
1	B	503	TRP	2.7
1	B	569	LYS	2.7
1	A	653	ASP	2.7
1	A	650	CYS	2.6
1	B	795	ASN	2.6
1	B	630	ALA	2.6
1	A	282	TYR	2.6
1	A	506	LYS	2.6
1	B	538	LYS	2.6
1	B	286	PHE	2.5
1	B	478	PHE	2.5
1	B	499	SER	2.5
1	B	1283	PHE	2.5
1	A	486	LEU	2.5
1	A	489	ILE	2.5
1	A	294	TYR	2.5
1	A	284	ALA	2.5
1	A	579	ASP	2.5
1	B	615	ASP	2.5
1	A	679	CYS	2.5
1	A	573	LEU	2.4
1	B	411	ASP	2.4
1	A	1246	ALA	2.4
1	A	600	THR	2.4
1	B	508	THR	2.4
1	B	792	ILE	2.4
1	A	413	THR	2.4
1	A	533	HIS	2.4
1	B	442	MET	2.4
1	B	445	LEU	2.4
1	A	357	PRO	2.4
1	A	669	VAL	2.4
1	B	362	PHE	2.4
1	B	1137	LYS	2.4
1	B	1057	GLN	2.4
1	B	1179	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	631	GLY	2.3
1	B	424	GLY	2.3
1	B	412	TYR	2.3
1	B	486	LEU	2.3
1	B	444	CYS	2.3
1	B	679	CYS	2.3
1	A	1241	ILE	2.3
1	A	1240	VAL	2.3
1	A	504	ASN	2.3
1	A	292	PHE	2.3
1	B	533	HIS	2.3
1	B	555	GLY	2.2
1	A	361	LYS	2.2
1	A	501	PRO	2.2
1	B	357	PRO	2.2
1	B	303	SER	2.2
1	B	481	GLU	2.2
1	B	285	THR	2.2
1	A	312	PHE	2.2
1	A	362	PHE	2.2
1	A	720	GLU	2.2
1	A	358	VAL	2.2
1	B	358	VAL	2.2
1	A	443	GLY	2.2
1	A	296	LEU	2.2
1	B	289	SER	2.2
1	A	1156	ALA	2.2
1	A	409	GLN	2.1
1	A	503	TRP	2.1
1	A	412	TYR	2.1
1	B	864	TYR	2.1
1	A	1024	ALA	2.1
1	B	598	VAL	2.1
1	B	471	LYS	2.1
1	A	285	THR	2.1
1	A	945	LEU	2.1
1	B	794	ILE	2.1
1	A	473	HIS	2.1
1	A	315	LEU	2.1
1	A	455	VAL	2.1
1	A	530	LYS	2.1
1	A	488	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	456	ARG	2.1
1	B	1241	ILE	2.1
1	A	535	LYS	2.0
1	B	1145	LYS	2.0
1	A	1057	GLN	2.0
1	B	1240	VAL	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](#)

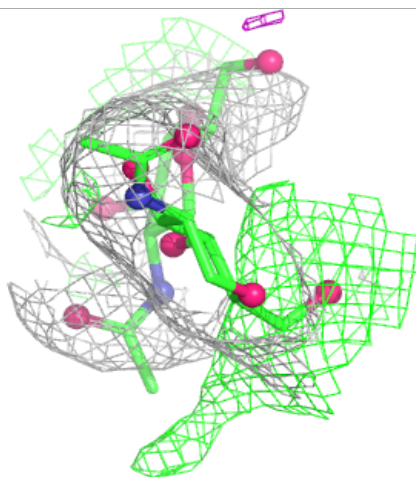
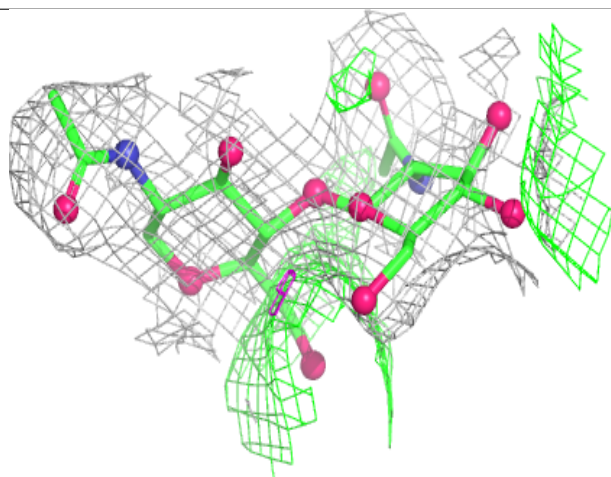
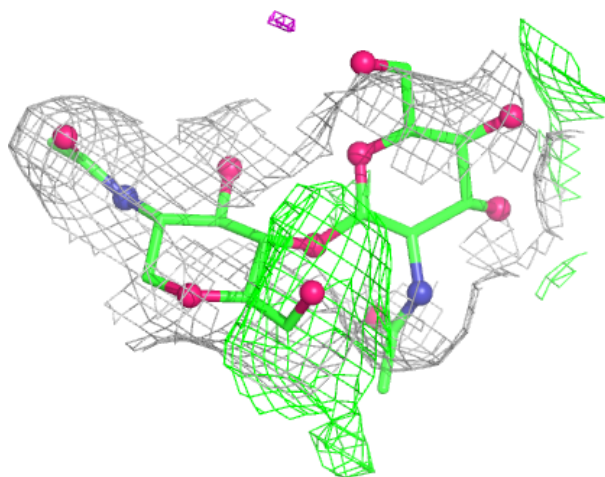
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

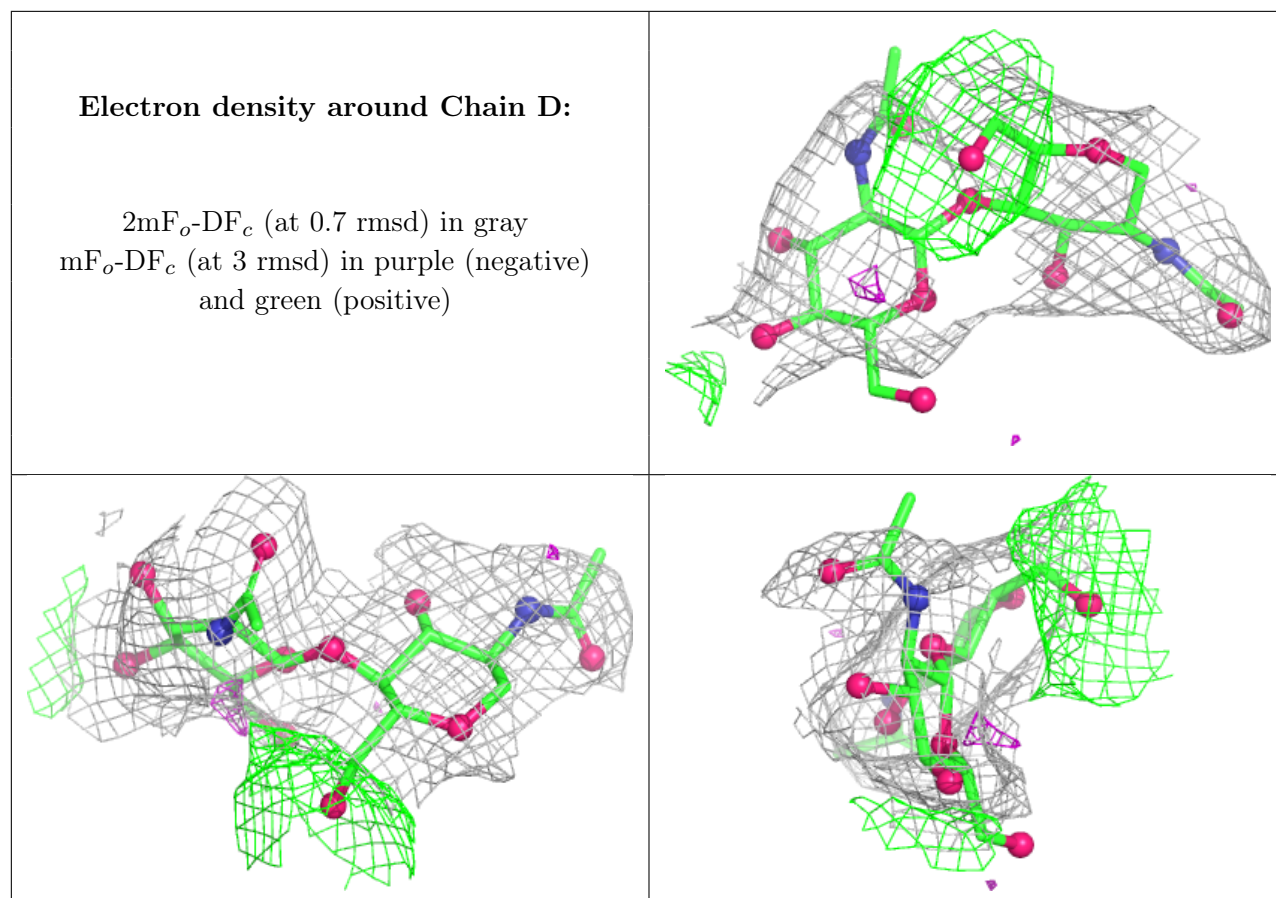
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	2	14/15	0.70	0.17	110,124,129,133	0
2	NAG	D	2	14/15	0.70	0.17	113,126,132,134	0
2	NAG	D	1	14/15	0.71	0.18	87,101,111,114	0
2	NAG	C	1	14/15	0.74	0.17	89,102,110,114	0

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)





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.