Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2023 – 11:58 PM EDT

PDB ID	:	3R05
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 (i) 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 (i)) were used in the production of this report:

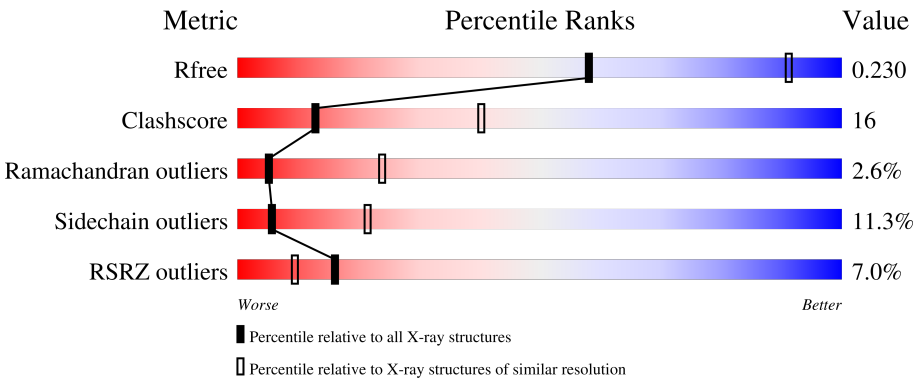
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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	6% 50% 24% 5% 20%
1	B	1254	5% 50% 24% 6% 20%
2	C	2	100%
2	D	2	50% 50%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	1008	7733	4857	1334	1499	43	0	0	0
1	B	1008	7733	4857	1334	1499	43	0	0	0

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.

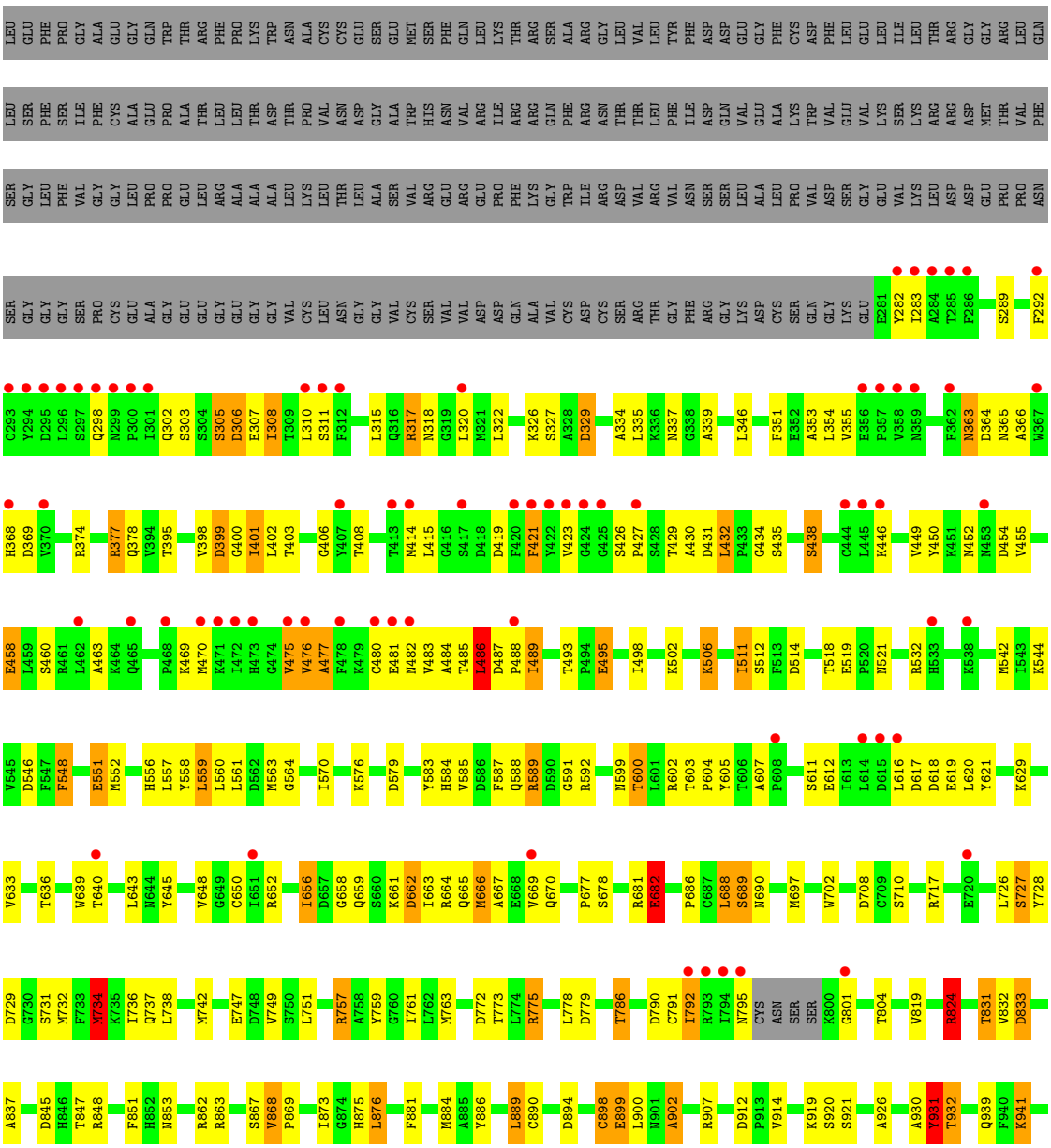
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
			Total	C	N	O			
2	D	2	28	16	2	10	0	0	0

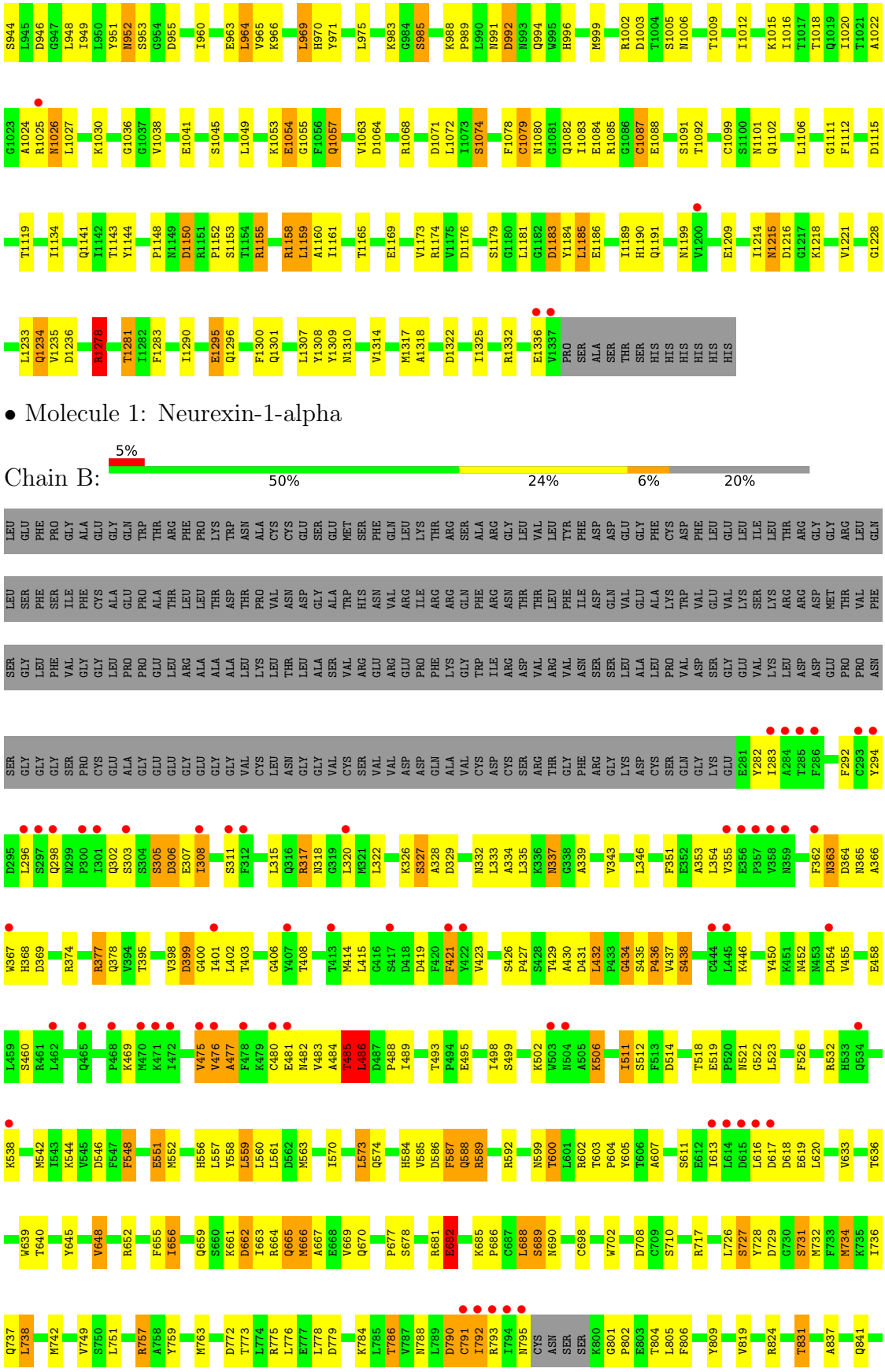
3 Residue-property plots (i)

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

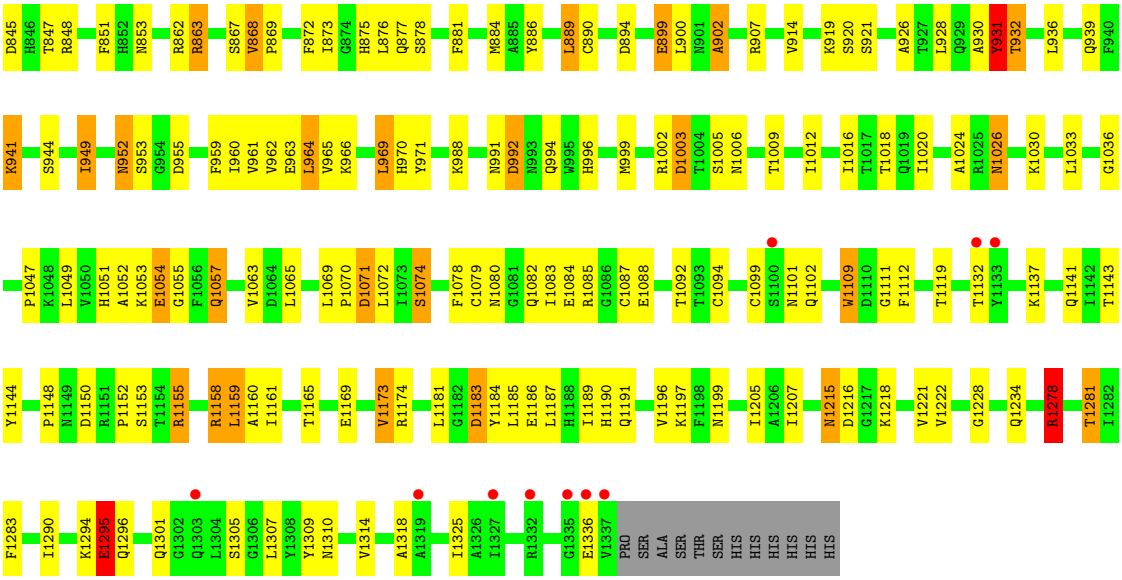
Chain A: 6% 50% 24% 5% 20%





- Molecule 1: Neurexin-1-alpha

Chain B:



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

Chain C: 100%

NAG1 NAG2

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

Chain D: 50% 50%

NAG1 NAG2

4 Data and refinement statistics (i)

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 – 2.94	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.29-2.95) 97.7 (44.29-2.94)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 2.96Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.235 0.202 , 0.230	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)	0.28 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.19	32/7886 (0.4%)	1.12	25/10691 (0.2%)
1	B	1.19	29/7886 (0.4%)	1.13	28/10691 (0.3%)
All	All	1.19	61/15772 (0.4%)	1.13	53/21382 (0.2%)

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 (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1057	GLN	CG-CD	14.07	1.83	1.51
1	B	1057	GLN	CG-CD	13.73	1.82	1.51
1	A	898	CYS	CB-SG	10.65	2.00	1.82
1	B	868	VAL	CB-CG2	-9.30	1.33	1.52
1	B	963	GLU	CD-OE2	9.26	1.35	1.25
1	A	963	GLU	CD-OE2	8.43	1.34	1.25
1	B	1054	GLU	CG-CD	8.29	1.64	1.51
1	A	1054	GLU	CG-CD	8.18	1.64	1.51
1	A	868	VAL	CB-CG2	-8.06	1.35	1.52
1	A	1036	GLY	C-O	7.79	1.36	1.23
1	A	1084	GLU	CD-OE1	7.48	1.33	1.25
1	A	899	GLU	CD-OE1	7.46	1.33	1.25
1	B	1094	CYS	CB-SG	-7.43	1.69	1.82
1	B	551	GLU	CG-CD	7.14	1.62	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1084	GLU	CD-OE1	7.07	1.33	1.25
1	A	1078	PHE	CE1-CZ	7.05	1.50	1.37
1	B	1295	GLU	CG-CD	6.99	1.62	1.51
1	A	1054	GLU	CD-OE1	6.87	1.33	1.25
1	B	931	TYR	CE2-CZ	6.84	1.47	1.38
1	B	1084	GLU	CD-OE2	6.83	1.33	1.25
1	A	551	GLU	CG-CD	6.68	1.61	1.51
1	A	931	TYR	CG-CD1	6.58	1.47	1.39
1	A	931	TYR	CE1-CZ	6.56	1.47	1.38
1	B	931	TYR	CE1-CZ	6.40	1.46	1.38
1	A	931	TYR	CE2-CZ	6.33	1.46	1.38
1	A	1038	VAL	CB-CG2	-6.30	1.39	1.52
1	A	1308	TYR	CD1-CE1	6.17	1.48	1.39
1	B	931	TYR	CG-CD1	6.16	1.47	1.39
1	A	963	GLU	CG-CD	6.15	1.61	1.51
1	A	1078	PHE	CB-CG	-6.15	1.40	1.51
1	B	1036	GLY	C-O	6.12	1.33	1.23
1	B	931	TYR	CD2-CE2	5.93	1.48	1.39
1	A	1057	GLN	CB-CG	5.89	1.68	1.52
1	B	1078	PHE	CD1-CE1	5.87	1.50	1.39
1	B	899	GLU	CD-OE1	5.85	1.32	1.25
1	B	1078	PHE	CE1-CZ	5.84	1.48	1.37
1	A	902	ALA	CA-CB	-5.80	1.40	1.52
1	A	1054	GLU	CD-OE2	5.77	1.31	1.25
1	A	951	TYR	CE1-CZ	-5.62	1.31	1.38
1	A	1099	CYS	CB-SG	5.62	1.91	1.82
1	B	890	CYS	CB-SG	-5.61	1.72	1.81
1	B	902	ALA	CA-CB	-5.61	1.40	1.52
1	B	872	PHE	CD1-CE1	-5.60	1.28	1.39
1	B	1054	GLU	CD-OE1	5.58	1.31	1.25
1	A	983	LYS	CD-CE	5.55	1.65	1.51
1	B	1109	TRP	CB-CG	-5.54	1.40	1.50
1	B	1057	GLN	CB-CG	5.51	1.67	1.52
1	B	926	ALA	CA-CB	-5.51	1.40	1.52
1	A	931	TYR	CD2-CE2	5.50	1.47	1.39
1	B	1099	CYS	CB-SG	5.50	1.91	1.82
1	B	1084	GLU	CG-CD	5.49	1.60	1.51
1	A	1084	GLU	CD-OE2	5.48	1.31	1.25
1	A	926	ALA	CA-CB	-5.40	1.41	1.52
1	B	1071	ASP	CB-CG	5.36	1.62	1.51
1	A	931	TYR	CD1-CE1	5.34	1.47	1.39
1	A	775	ARG	CG-CD	5.29	1.65	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	809	TYR	CB-CG	-5.29	1.43	1.51
1	A	1079	CYS	CB-SG	-5.28	1.73	1.81
1	A	931	TYR	CG-CD2	5.27	1.46	1.39
1	B	992	ASP	CB-CG	5.22	1.62	1.51
1	A	761	ILE	C-O	5.10	1.33	1.23

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1071	ASP	CB-CG-OD1	10.07	127.37	118.30
1	A	824	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	B	1053	LYS	CD-CE-NZ	-9.41	90.05	111.70
1	A	941	LYS	CD-CE-NZ	-8.72	91.65	111.70
1	A	824	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	B	941	LYS	CD-CE-NZ	-8.52	92.11	111.70
1	B	306	ASP	CB-CG-OD2	8.51	125.95	118.30
1	A	1053	LYS	CD-CE-NZ	-8.16	92.92	111.70
1	A	876	LEU	CB-CG-CD1	-7.89	97.59	111.00
1	A	1087	CYS	CA-CB-SG	-7.59	100.33	114.00
1	B	486	LEU	CA-CB-CG	6.88	131.13	115.30
1	A	486	LEU	CA-CB-CG	6.82	130.99	115.30
1	A	999	MET	CG-SD-CE	6.72	110.95	100.20
1	A	559	LEU	CA-CB-CG	-6.50	100.34	115.30
1	A	1119	THR	C-N-CA	-6.47	105.52	121.70
1	B	863	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	B	698	CYS	CA-CB-SG	-6.19	102.85	114.00
1	A	890	CYS	CA-CB-SG	-6.18	102.87	114.00
1	B	801	GLY	N-CA-C	-6.11	97.82	113.10
1	B	757	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	890	CYS	CA-CB-SG	-5.92	103.34	114.00
1	B	960	ILE	CG1-CB-CG2	-5.89	98.44	111.40
1	A	757	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	964	LEU	CA-CB-CG	-5.83	101.90	115.30
1	B	775	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	819	VAL	CB-CA-C	-5.79	100.40	111.40
1	B	1158	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	B	1119	THR	C-N-CA	-5.64	107.59	121.70
1	A	1064	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	1278	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	1003	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	960	ILE	CG1-CB-CG2	-5.57	99.14	111.40
1	B	889	LEU	CA-CB-CG	-5.53	102.59	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	738	LEU	CA-CB-CG	-5.51	102.62	115.30
1	A	975	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	B	969	LEU	CB-CG-CD1	-5.39	101.84	111.00
1	A	964	LEU	CA-CB-CG	-5.38	102.94	115.30
1	B	999	MET	CG-SD-CE	5.36	108.78	100.20
1	A	889	LEU	CA-CB-CG	-5.36	102.98	115.30
1	B	992	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	485	THR	N-CA-C	5.34	125.43	111.00
1	B	889	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	A	992	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	1158	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	A	863	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	B	1278	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	912	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	801	GLY	N-CA-C	-5.18	100.14	113.10
1	B	949	ILE	CG1-CB-CG2	-5.18	100.00	111.40
1	A	734	MET	CG-SD-CE	5.18	108.48	100.20
1	B	779	ASP	CB-CG-OD1	5.15	122.93	118.30
1	B	819	VAL	CB-CA-C	-5.08	101.74	111.40
1	B	559	LEU	CA-CB-CG	-5.07	103.64	115.30

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
1	B	484	ALA	Peptide
1	B	790	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7733	0	7482	253	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7733	0	7482	260	0
2	C	28	0	25	0	0
2	D	28	0	25	4	0
All	All	15522	0	15014	503	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 16.

All (503) 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	1.46
1:A:1057:GLN:CD	1:A:1057:GLN:CG	1.83	1.44
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
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:B:751:LEU:C	1:B:751:LEU:HD12	2.00	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:B:519:GLU:HG3	1:B:648:VAL:CG2	2.12	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:688:LEU:C	1:A:690:ASN:H	1.89	0.75
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:B:305:SER:O	1:B:306:ASP:HB3	1.88	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
1:A:452:ASN:ND2	1:A:454:ASP:H	1.88	0.70
1:B:318:ASN:HA	1:B:335:LEU:O	1.91	0.70
1:A:430:ALA:HB2	1:A:438:SER:HB3	1.71	0.70
1:B:431:ASP:O	1:B:432:LEU:C	2.29	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: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:751:LEU:HD12	1:A:751:LEU:C	2.15	0.67
1:B:306:ASP:OD2	1:B:374:ARG:HD3	1.95	0.67
1:B:587:PHE:CD1	1:B:587:PHE:C	2.66	0.67
1:A:302:GLN:HA	1:A:415:LEU:O	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:GLN:HA	1:B:415:LEU:O	1.94	0.66
1:B:688:LEU:C	1:B:690:ASN:H	1.96	0.66
1:A:688:LEU:C	1:A:690:ASN:N	2.47	0.66
1:B:587:PHE:C	1:B:587:PHE:HD1	1.99	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: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: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: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: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
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:727:SER:HB2	1:A:875:HIS:HD2	1.55	0.63
1:B:1159:LEU:C	1:B:1159:LEU:HD23	2.19	0.63
1:A:431:ASP:O	1:A:432:LEU:C	2.35	0.62
1:A:429:THR:HG22	1:A:438:SER:HA	1.79	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: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:B:688:LEU:C	1:B:690:ASN:N	2.52	0.61
1:A:369:ASP:HB2	1:A:399:ASP:HA	1.83	0.61
1:B:311:SER:HB2	1:B:446:LYS:HB3	1.82	0.61
1:B:952:ASN:HD22	1:B:952:ASN:C	2.04	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1184:TYR:CD1	1:B:1184:TYR:C	2.74	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: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:548:PHE:CD2	1:A:548:PHE:C	2.71	0.59
1:A:757:ARG:HD2	1:A:873:ILE:HD12	1.84	0.59
1:B:512:SER:HA	1:B:585:VAL:O	2.02	0.59
1:B:751:LEU:C	1:B:751:LEU:CD1	2.71	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:A:663:ILE:C	1:A:665:GLN:H	2.06	0.58
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:A:563:MET:HE1	1:A:607:ALA:HB3	1.85	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
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:1025:ARG:HD2	2:D:1:NAG:C8	2.32	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:A:1296:GLN:CD	1:A:1296:GLN:H	2.08	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:1159:LEU:HD23	1:A:1159:LEU:C	2.26	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:LEU:CD2	1:A:894:ASP:HB2	2.35	0.56
1:A:1184:TYR:CD1	1:A:1184:TYR:C	2.79	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: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:B:663:ILE:C	1:B:665:GLN:H	2.09	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
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: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: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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1112:PHE:CD1	1:A:1112:PHE:C	2.83	0.52
1:B:969:LEU:CD2	1:B:1012:ILE:HD11	2.39	0.52
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: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: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:663:ILE:C	1:A:665:GLN:N	2.64	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:959:PHE:CD1	1:B:959:PHE:C	2.84	0.49
1:B:1020:ILE:O	1:B:1020:ILE:CG2	2.60	0.49
1:B:1112:PHE:CD1	1:B:1112:PHE:C	2.86	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:663:ILE:C	1:B:665:GLN:N	2.66	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:734:MET:HE3	1:B:736:ILE:HD12	1.93	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:A:493:THR:C	1:A:648:VAL:HG12	2.33	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:A:737:GLN:O	1:A:738:LEU:C	2.51	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1165:THR:O	1:A:1215:ASN:HA	2.14	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:A:681:ARG:HG3	1:A:702:TRP:CH2	2.48	0.48
1:B:320:LEU:HA	1:B:334:ALA:HB2	1.95	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:B:1296:GLN:CD	1:B:1296:GLN:H	2.17	0.48
1:A:728:TYR:HE2	1:A:876:LEU:HD12	1.75	0.48
1:A:751:LEU:C	1:A:751:LEU:CD1	2.81	0.48
1:A:952:ASN:HD22	1:A:952:ASN:C	2.17	0.48
1:B:476:VAL:O	1:B:477:ALA:CB	2.62	0.48
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: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:B:1159:LEU:C	1:B:1159:LEU:CD2	2.83	0.47
1:A:311:SER:HA	1:A:368:HIS:O	2.15	0.47
1:A:587:PHE:CD1	1:A:587:PHE:C	2.83	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:N	1:B:845:ASP:OD1	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: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:737:GLN:O	1:B:738:LEU:C	2.51	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:1155:ARG:HH11	1:B:1155:ARG:CG	2.18	0.46
1:A:1003:ASP:OD1	1:A:1003:ASP:C	2.54	0.46
1:A:1296:GLN:CD	1:A:1296:GLN:N	2.68	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: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: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: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:868:VAL:O	1:A:869:PRO:C	2.53	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1005:SER:O	1:A:1006:ASN:HB2	2.17	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:1317:MET:HE3	1:A:1322:ASP:OD1	2.17	0.45
1:B:322:LEU:HD12	1:B:421:PHE:HE1	1.81	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: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:B:308:ILE:HD13	1:B:450:TYR:HD1	1.82	0.44
1:A:1158:ARG:HH11	1:A:1158:ARG:HD2	1.55	0.44
1:B:1003:ASP:C	1:B:1003:ASP:OD1	2.55	0.44
1:A:736:ILE:HG12	1:A:886:TYR:CD2	2.52	0.44
1:A:557:LEU:HG	1:A:558:TYR:N	2.33	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: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:681:ARG:O	1:B:682:GLU:C	2.56	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:B:557:LEU:HG	1:B:558:TYR:N	2.33	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1173:VAL:HG13	1:B:1187:LEU:HB3	2.01	0.43
1:A:398:VAL:C	1:A:400:GLY:H	2.21	0.43
1:A:734:MET:HE3	1:A:736:ILE:HD12	2.01	0.43
1:A:1016:ILE:HG22	1:A:1018:THR:HG23	2.00	0.43
1:A:1309:TYR:O	1:A:1310:ASN:C	2.56	0.43
1:B:298:GLN:HG2	1:B:469:LYS:HE3	2.01	0.43
1:B:436:PRO:HD2	1:B:437:VAL:H	1.83	0.43
1:A:548:PHE:HD1	1:A:587:PHE:HE2	1.64	0.43
1:A:681:ARG:O	1:A:682:GLU:C	2.56	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:A:1159:LEU:C	1:A:1159:LEU:CD2	2.86	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:B:961:VAL:CG1	1:B:962:VAL:N	2.82	0.43
1:B:1309:TYR:O	1:B:1310:ASN:C	2.57	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: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: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: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:988:LYS:CD	1:B:731:SER:HB3	2.49	0.42
1:B:398:VAL:C	1:B:400:GLY:H	2.23	0.42
1:A:791:CYS:O	1:A:792:ILE:HB	2.19	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1296:GLN:CD	1:B:1296:GLN:N	2.73	0.42
1:A:495:GLU:OE2	1:A:495:GLU:N	2.51	0.42
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: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:A:985:SER:HG	1:B:1109:TRP:HE1	1.67	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:A:779:ASP:C	1:A:779:ASP:OD1	2.59	0.41
1:B:488:PRO:HB3	1:B:652:ARG:CB	2.46	0.41
1:B:322:LEU:CD2	1:B:333:LEU:HD23	2.50	0.41
1:B:1087:CYS:O	1:B:1087:CYS:SG	2.79	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:398:VAL:C	1:A:400:GLY:N	2.73	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: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:A:1214:ILE:C	1:A:1214:ILE:HD12	2.41	0.41
1:B:563:MET:HE1	1:B:607:ALA:HB3	2.01	0.41
1:B:790:ASP:OD2	1:B:791:CYS:N	2.44	0.41
1:A:1228:GLY:CA	1:A:1281:THR:HG22	2.43	0.41
1:A:643:LEU:HD21	1:A:824:ARG:NH2	2.36	0.40
1:A:662:ASP:O	1:A:666:MET:HE2	2.22	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:A:400:GLY:O	1:A:401:ILE:CB	2.69	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:MET:HE2	1:B:607:ALA:HB3	2.00	0.40
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:A:1300:PHE:CG	1:A:1301:GLN:N	2.89	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:B:1051:HIS:O	1:B:1052:ALA:C	2.60	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:1024:ALA:O	1:A:1025:ARG:C	2.59	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: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:B:362:PHE:C	1:B:364:ASP:H	2.24	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%)	5 24
1	B	1004/1254 (80%)	881 (88%)	96 (10%)	27 (3%)	5 23
All	All	2008/2508 (80%)	1762 (88%)	193 (10%)	53 (3%)	5 24

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	337	ASN
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%)	742 (88%)	97 (12%)	5 20
1	B	839/1068 (79%)	747 (89%)	92 (11%)	6 22
All	All	1678/2136 (79%)	1489 (89%)	189 (11%)	6 21

All (189) 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	329	ASP
1	A	365	ASN
1	A	377	ARG
1	A	402	LEU
1	A	419	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	421	PHE
1	A	432	LEU
1	A	438	SER
1	A	455	VAL
1	A	458	GLU
1	A	482	ASN
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	546	ASP
1	A	548	PHE
1	A	561	LEU
1	A	588	GLN
1	A	589	ARG
1	A	592	ARG
1	A	611	SER
1	A	616	LEU
1	A	617	ASP
1	A	620	LEU
1	A	633	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	763	MET
1	A	773	THR
1	A	786	THR
1	A	795	ASN
1	A	824	ARG
1	A	831	THR
1	A	847	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	853	ASN
1	A	862	ARG
1	A	867	SER
1	A	898	CYS
1	A	899	GLU
1	A	907	ARG
1	A	914	VAL
1	A	931	TYR
1	A	932	THR
1	A	941	LYS
1	A	944	SER
1	A	952	ASN
1	A	969	LEU
1	A	971	TYR
1	A	985	SER
1	A	989	PRO
1	A	1026	ASN
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	1150	ASP
1	A	1153	SER
1	A	1155	ARG
1	A	1159	LEU
1	A	1173	VAL
1	A	1176	ASP
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	1283	PHE
1	A	1295	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	365	ASN
1	B	377	ARG
1	B	402	LEU
1	B	419	ASP
1	B	421	PHE
1	B	432	LEU
1	B	438	SER
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	498	ILE
1	B	499	SER
1	B	506	LYS
1	B	511	ILE
1	B	518	THR
1	B	542	MET
1	B	546	ASP
1	B	548	PHE
1	B	561	LEU
1	B	587	PHE
1	B	588	GLN
1	B	589	ARG
1	B	592	ARG
1	B	611	SER
1	B	616	LEU
1	B	617	ASP
1	B	620	LEU
1	B	633	VAL
1	B	648	VAL
1	B	656	ILE
1	B	662	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	665	GLN
1	B	678	SER
1	B	682	GLU
1	B	688	LEU
1	B	717	ARG
1	B	727	SER
1	B	731	SER
1	B	734	MET
1	B	763	MET
1	B	773	THR
1	B	786	THR
1	B	795	ASN
1	B	831	THR
1	B	847	THR
1	B	853	ASN
1	B	862	ARG
1	B	863	ARG
1	B	867	SER
1	B	899	GLU
1	B	907	ARG
1	B	914	VAL
1	B	931	TYR
1	B	932	THR
1	B	941	LYS
1	B	944	SER
1	B	952	ASN
1	B	971	TYR
1	B	1026	ASN
1	B	1049	LEU
1	B	1054	GLU
1	B	1074	SER
1	B	1079	CYS
1	B	1082	GLN
1	B	1085	ARG
1	B	1088	GLU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1186	GLU
1	B	1221	VAL
1	B	1234	GLN
1	B	1278	ARG
1	B	1281	THR
1	B	1283	PHE
1	B	1294	LYS
1	B	1295	GLU
1	B	1336	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	365	ASN
1	A	452	ASN
1	A	788	ASN
1	A	952	ASN
1	A	994	GLN
1	A	1301	GLN
1	A	1321	ASN
1	B	365	ASN
1	B	378	GLN
1	B	440	ASN
1	B	452	ASN
1	B	588	GLN
1	B	743	HIS
1	B	788	ASN
1	B	952	ASN
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	2,1	14,14,15	0.88	0	17,19,21	2.97	10 (58%)
2	NAG	C	2	2	14,14,15	0.61	0	17,19,21	1.72	3 (17%)
2	NAG	D	1	2,1	14,14,15	0.84	0	17,19,21	3.05	9 (52%)
2	NAG	D	2	2	14,14,15	0.81	1 (7%)	17,19,21	1.60	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	2,1	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	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	2.06	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	NAG	C1-O5-C5	7.00	121.67	112.19
2	C	1	NAG	C1-O5-C5	6.05	120.39	112.19
2	C	1	NAG	O5-C5-C6	4.63	114.46	107.20
2	C	2	NAG	O5-C5-C6	4.53	114.30	107.20
2	D	1	NAG	O5-C5-C6	4.49	114.24	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	NAG	O5-C5-C6	4.41	114.12	107.20
2	C	1	NAG	O7-C7-C8	-4.24	114.19	122.06
2	D	1	NAG	C2-N2-C7	4.11	128.76	122.90
2	D	1	NAG	C1-C2-N2	4.08	117.45	110.49
2	C	1	NAG	C1-C2-N2	3.93	117.21	110.49
2	D	1	NAG	O7-C7-C8	-3.57	115.43	122.06
2	C	1	NAG	C2-N2-C7	3.39	127.73	122.90
2	D	1	NAG	O7-C7-N2	3.20	127.83	121.95
2	D	1	NAG	O4-C4-C3	-3.02	103.38	110.35
2	C	1	NAG	O4-C4-C3	-2.91	103.63	110.35
2	C	1	NAG	C4-C3-C2	2.88	115.24	111.02
2	C	1	NAG	O7-C7-N2	2.82	127.14	121.95
2	C	2	NAG	C1-O5-C5	-2.76	108.45	112.19
2	C	1	NAG	C6-C5-C4	2.61	119.12	113.00
2	D	1	NAG	O6-C6-C5	2.60	120.21	111.29
2	C	2	NAG	C2-N2-C7	-2.38	119.51	122.90
2	D	2	NAG	C1-O5-C5	-2.36	108.99	112.19
2	D	2	NAG	C4-C3-C2	2.35	114.46	111.02
2	C	1	NAG	O6-C6-C5	2.28	119.12	111.29
2	D	1	NAG	C6-C5-C4	2.12	117.96	113.00
2	D	2	NAG	C2-N2-C7	-2.05	119.99	122.90

There are no chirality outliers.

All (6) 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	D	1	NAG	O5-C5-C6-O6

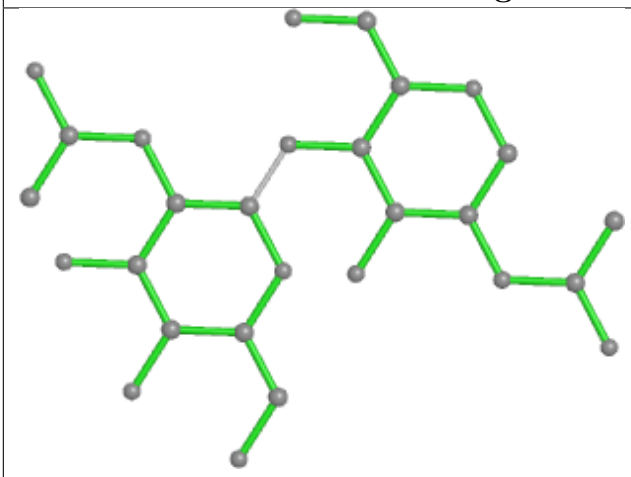
There are no ring outliers.

1 monomer is involved in 4 short contacts:

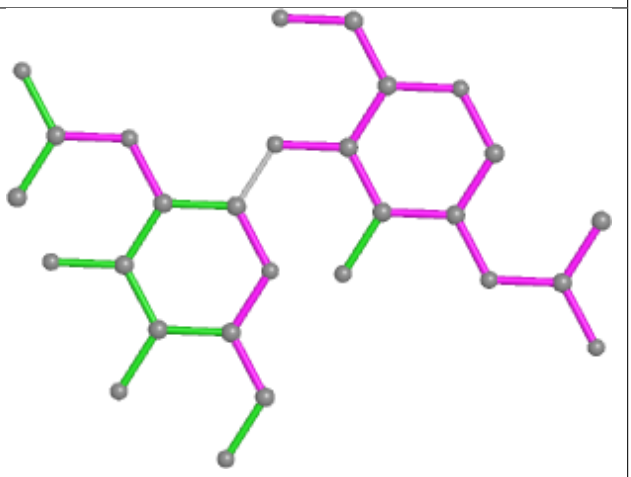
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	4	0

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

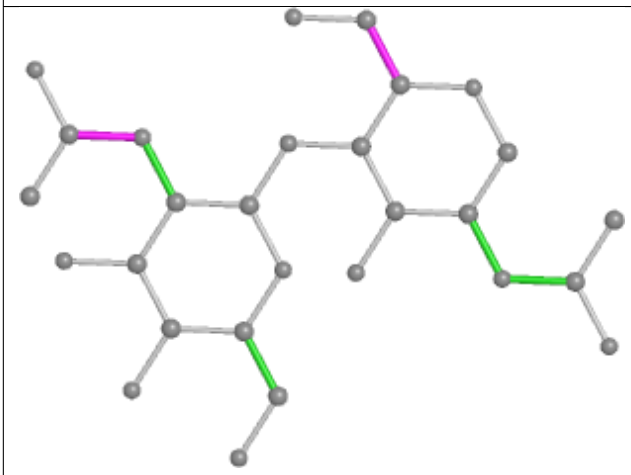
Oligosaccharide Chain C



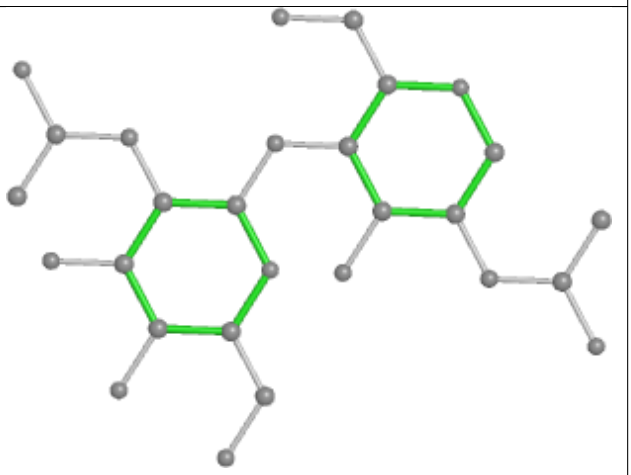
Bond lengths



Bond angles

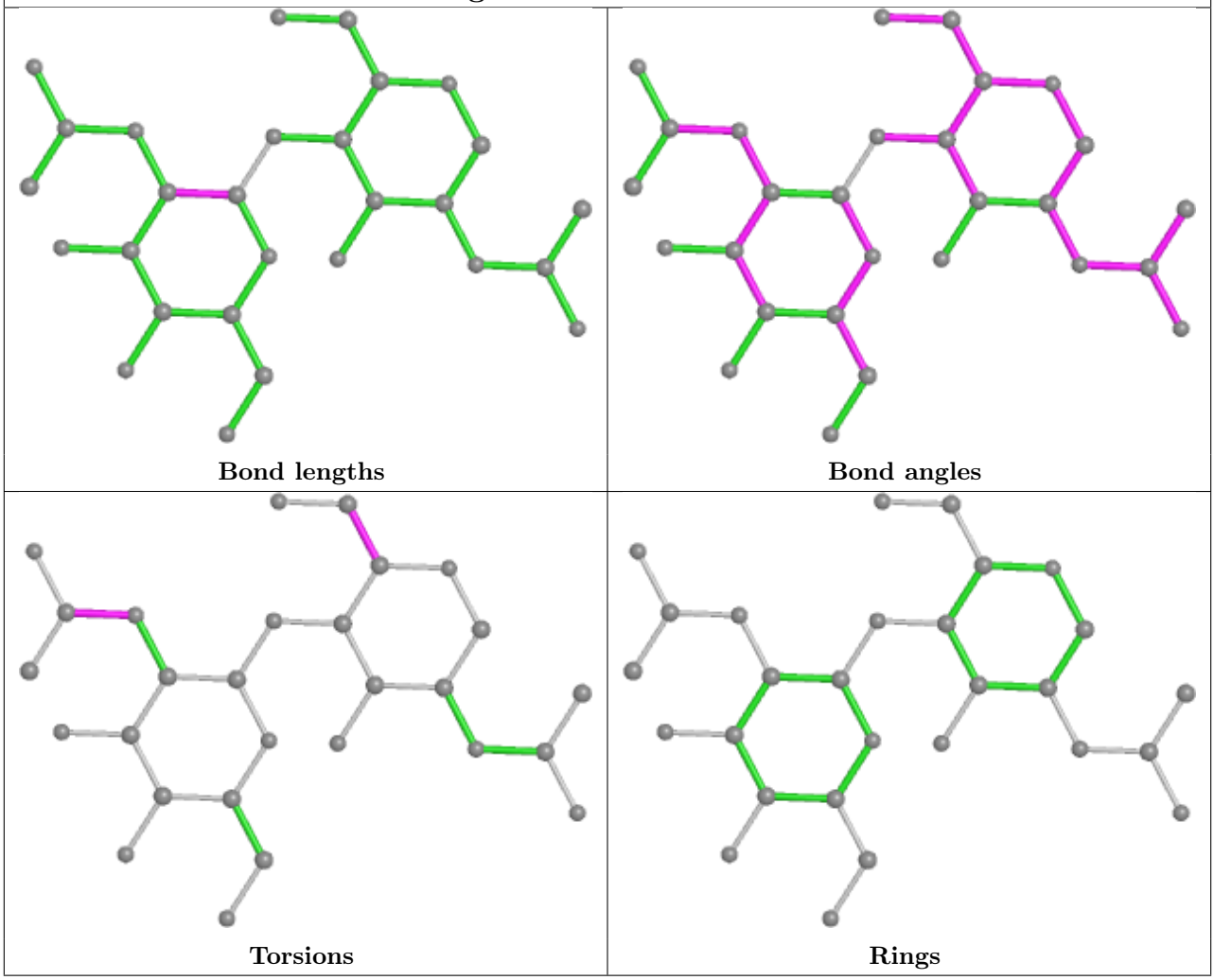


Torsions



Rings

Oligosaccharide Chain D



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.20	75 (7%) 14 8	35, 91, 151, 196	0
1	B	1008/1254 (80%)	0.20	67 (6%) 18 10	34, 92, 152, 201	0
All	All	2016/2508 (80%)	0.20	142 (7%) 16 9	34, 91, 152, 201	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	472	ILE	5.9
1	B	358	VAL	5.7
1	A	359	ASN	5.7
1	B	284	ALA	5.5
1	A	480	CYS	5.5
1	B	445	LEU	5.4
1	A	358	VAL	5.2
1	B	794	ILE	5.2
1	A	294	TYR	5.1
1	A	445	LEU	4.9
1	A	300	PRO	4.9
1	A	1337	VAL	4.8
1	A	481	GLU	4.7
1	A	284	ALA	4.6
1	A	296	LEU	4.6
1	A	478	PHE	4.6
1	B	359	ASN	4.6
1	A	293	CYS	4.3
1	A	425	GLY	4.1
1	A	444	CYS	4.0
1	B	481	GLU	3.9
1	B	614	LEU	3.9
1	A	295	ASP	3.9
1	B	476	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1335	GLY	3.7
1	B	312	PHE	3.7
1	A	312	PHE	3.7
1	A	357	PRO	3.7
1	B	301	ILE	3.7
1	B	478	PHE	3.6
1	B	615	ASP	3.6
1	A	301	ILE	3.6
1	B	795	ASN	3.6
1	A	417	SER	3.4
1	A	283	ILE	3.4
1	A	311	SER	3.4
1	B	311	SER	3.4
1	A	362	PHE	3.4
1	A	367	TRP	3.4
1	A	462	LEU	3.3
1	B	470	MET	3.3
1	B	294	TYR	3.3
1	B	293	CYS	3.2
1	B	283	ILE	3.2
1	A	356	GLU	3.2
1	B	1337	VAL	3.1
1	A	795	ASN	3.1
1	A	320	LEU	3.1
1	A	538	LYS	3.1
1	A	470	MET	3.1
1	A	472	ILE	3.1
1	A	422	TYR	3.1
1	A	297	SER	3.1
1	A	794	ILE	3.1
1	A	423	VAL	3.0
1	B	367	TRP	3.0
1	B	413	THR	3.0
1	B	538	LYS	3.0
1	B	357	PRO	3.0
1	B	444	CYS	3.0
1	B	286	PHE	2.9
1	A	488	PRO	2.9
1	A	615	ASP	2.9
1	B	1303	GLN	2.9
1	A	285	THR	2.8
1	B	308	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1025	ARG	2.8
1	B	616	LEU	2.8
1	A	424	GLY	2.7
1	B	613	ILE	2.7
1	B	362	PHE	2.7
1	B	480	CYS	2.7
1	B	1319	ALA	2.7
1	B	462	LEU	2.7
1	B	1336	GLU	2.7
1	A	310	LEU	2.7
1	A	286	PHE	2.6
1	B	417	SER	2.6
1	A	298	GLN	2.6
1	A	468	PRO	2.6
1	A	471	LYS	2.6
1	A	482	ASN	2.6
1	B	1133	TYR	2.5
1	A	614	LEU	2.5
1	A	475	VAL	2.5
1	B	356	GLU	2.5
1	A	651	ILE	2.5
1	A	1200	VAL	2.4
1	A	465	GLN	2.4
1	A	420	PHE	2.4
1	A	476	VAL	2.4
1	B	1100	SER	2.4
1	A	616	LEU	2.4
1	B	407	TYR	2.4
1	B	421	PHE	2.4
1	A	299	ASN	2.4
1	A	792	ILE	2.4
1	B	792	ILE	2.4
1	A	1336	GLU	2.4
1	A	407	TYR	2.4
1	B	504	ASN	2.4
1	A	453	ASN	2.3
1	B	320	LEU	2.3
1	A	292	PHE	2.3
1	A	669	VAL	2.3
1	B	793	ARG	2.3
1	B	791	CYS	2.3
1	A	368	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	801	GLY	2.3
1	B	534	GLN	2.3
1	B	1332	ARG	2.3
1	B	422	TYR	2.3
1	B	465	GLN	2.3
1	B	475	VAL	2.3
1	A	414	MET	2.3
1	A	421	PHE	2.3
1	B	298	GLN	2.2
1	B	1132	THR	2.2
1	A	720	GLU	2.2
1	A	793	ARG	2.2
1	B	468	PRO	2.2
1	B	454	ASP	2.2
1	A	533	HIS	2.2
1	B	285	THR	2.2
1	A	427	PRO	2.2
1	B	471	LYS	2.1
1	B	617	ASP	2.1
1	B	503	TRP	2.1
1	A	473	HIS	2.1
1	B	303	SER	2.1
1	A	413	THR	2.1
1	B	355	VAL	2.1
1	B	300	PRO	2.1
1	A	640	THR	2.1
1	B	297	SER	2.1
1	A	282	TYR	2.1
1	B	1327	ILE	2.1
1	B	296	LEU	2.0
1	B	401	ILE	2.0
1	A	608	PRO	2.0
1	A	370	VAL	2.0
1	A	446	LYS	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)

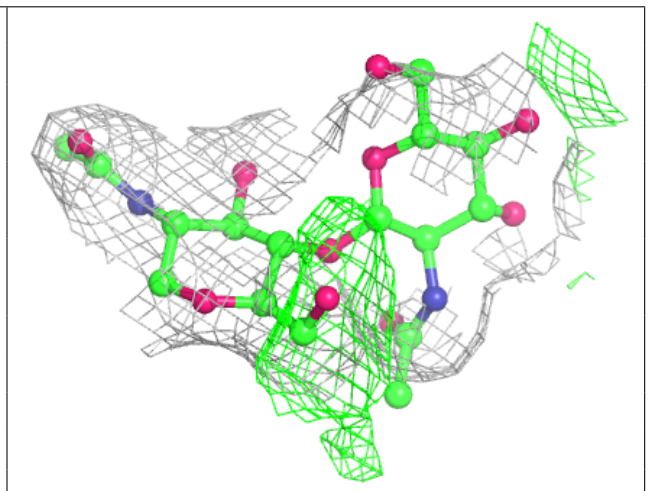
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

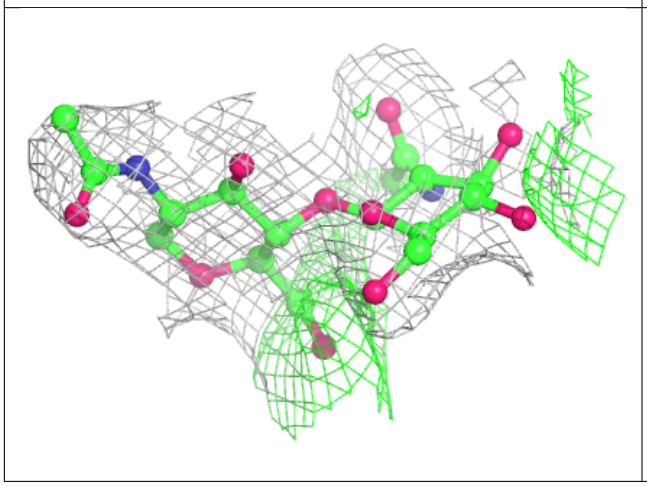
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	D	2	14/15	0.82	0.33	113,126,132,134	0
2	NAG	C	2	14/15	0.84	0.23	110,124,129,133	0
2	NAG	D	1	14/15	0.85	0.18	87,101,111,114	0
2	NAG	C	1	14/15	0.86	0.16	89,102,110,114	0

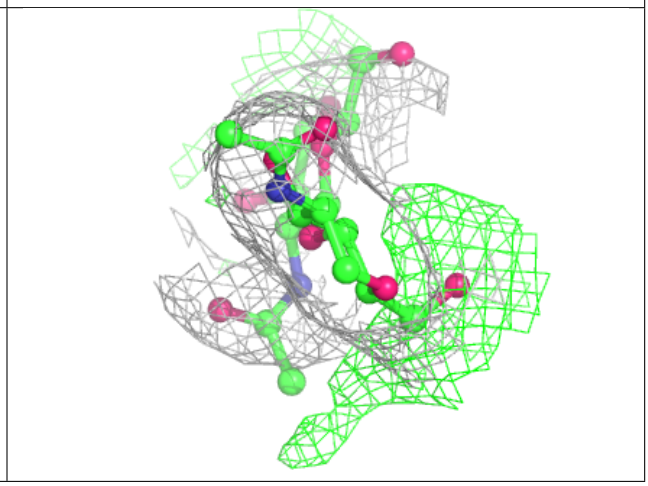
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

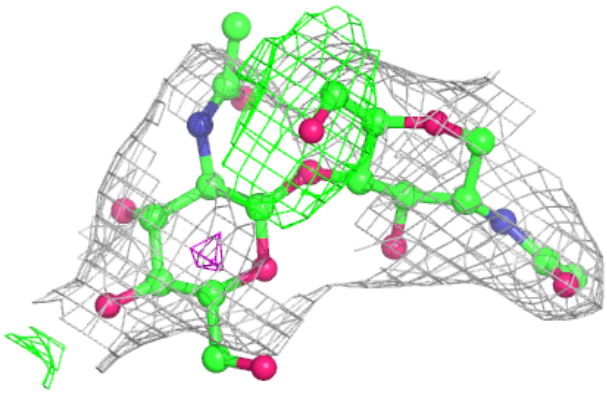


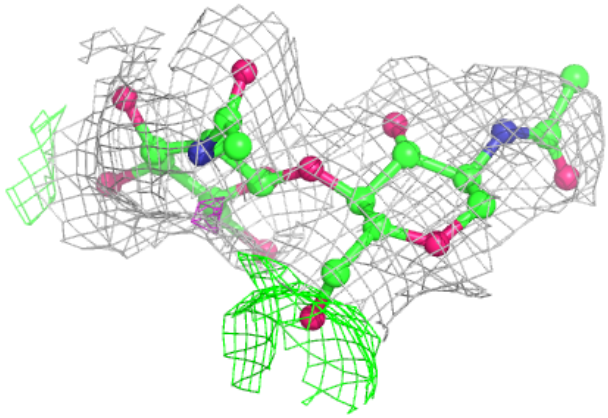


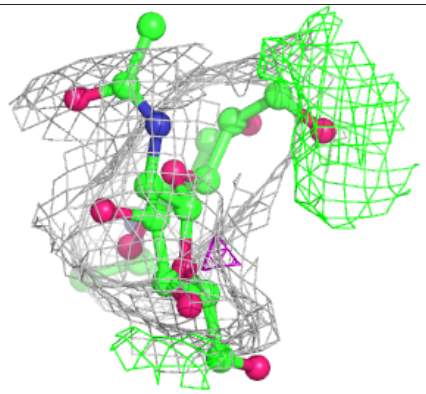


Electron density around Chain D:

$2mF_o$-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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.