



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:00 PM UTC

PDB ID : 2D04 / pdb_00002d04
Title : Crystal structure of neoculin, a sweet protein with taste-modifying activity.
Authors : Shimizu-Ibuka, A.; Morita, Y.; Terada, T.; Asakura, T.; Nakajima, K.; Iwata, S.; Misaka, T.; Sorimachi, H.; Arai, S.; Abe, K.
Deposited on : 2005-07-25
Resolution : 2.76 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

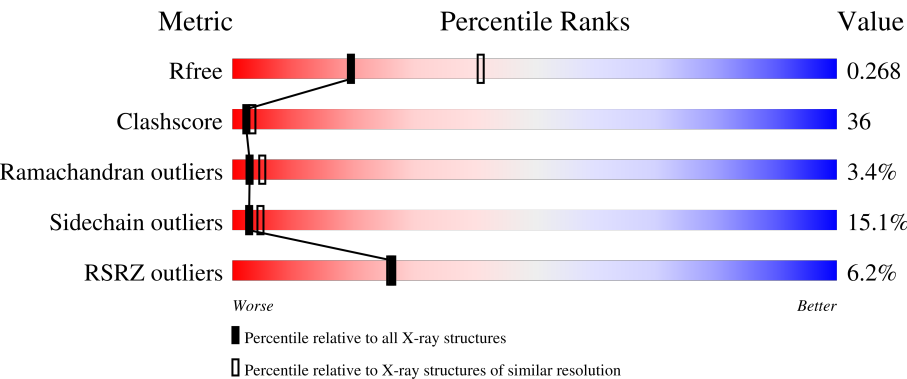
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	113	4% 34% 48% 13% . .
1	C	113	8% 43% 42% 12% .
1	E	113	8% 36% 42% 18% . .
1	G	113	6% 39% 43% 13% . .
2	B	114	6% 35% 46% 11% 5% .

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Mol	Chain	Length	Quality of chain
2	D	114	2% 35%47%10%5%•
2	F	114	7% 35%46%13%••
2	H	114	8% 36%39%19%••
3	I	4	50%50%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7112 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.

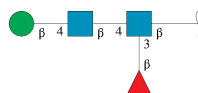
- Molecule 1 is a protein called neoculin acidic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			855	534	149	167	5			
1	C	113	Total	C	N	O	S	0	0	0
			872	544	152	171	5			
1	E	111	Total	C	N	O	S	0	0	0
			855	534	149	167	5			
1	G	110	Total	C	N	O	S	0	0	0
			849	531	148	165	5			

- Molecule 2 is a protein called Curculin.

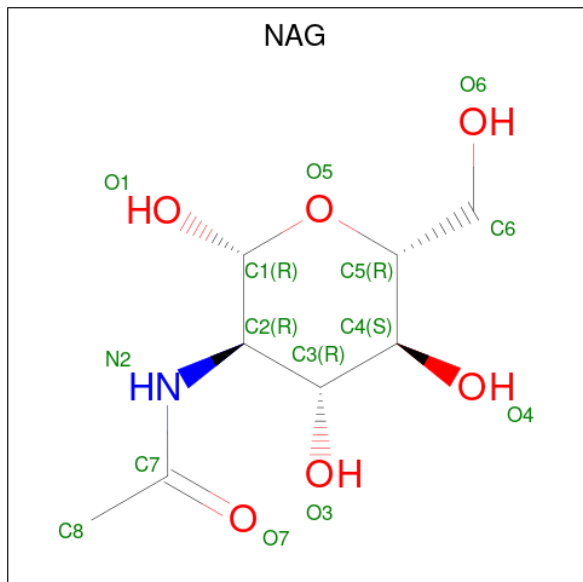
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	111	Total	C	N	O	S	0	0	0
			866	538	163	161	4			
2	D	111	Total	C	N	O	S	0	0	0
			866	538	163	161	4			
2	F	110	Total	C	N	O	S	0	0	0
			855	532	159	160	4			
2	H	111	Total	C	N	O	S	3	0	0
			866	538	163	161	4			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

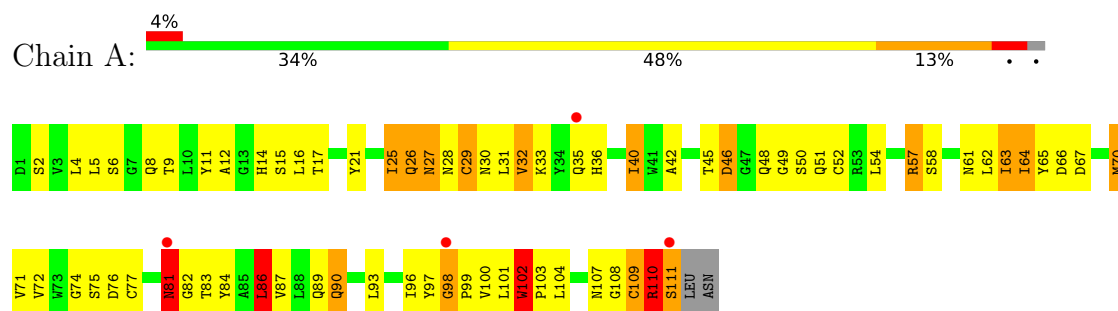
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total	O	0	0
			27	27		
5	B	18	Total	O	0	0
			18	18		
5	C	24	Total	O	0	0
			24	24		
5	D	24	Total	O	0	0
			24	24		
5	E	19	Total	O	0	0
			19	19		
5	F	17	Total	O	0	0
			17	17		
5	G	15	Total	O	0	0
			15	15		
5	H	21	Total	O	0	0
			21	21		

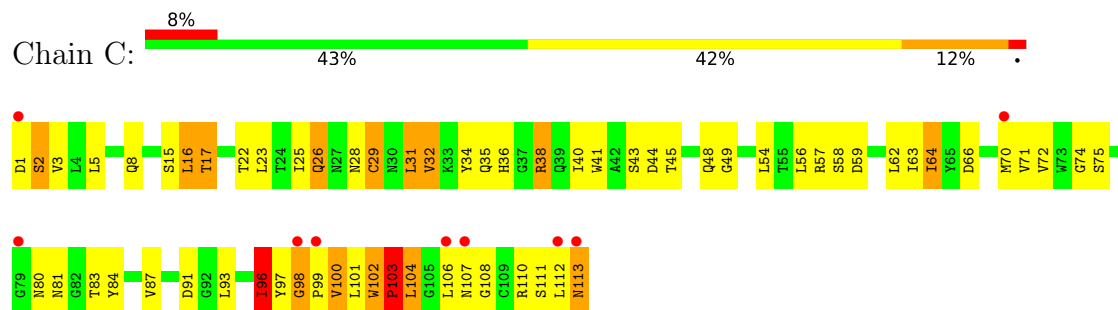
3 Residue-property plots [i](#)

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.

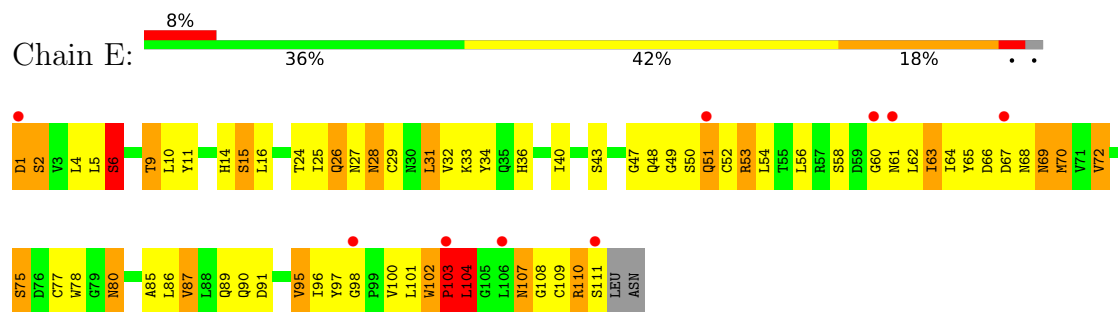
• Molecule 1: neoculin acidic subunit



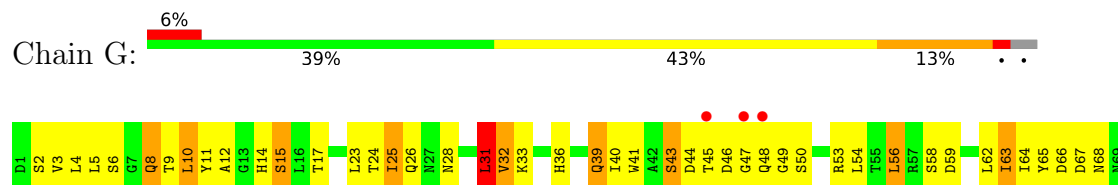
• Molecule 1: neoculin acidic subunit



• Molecule 1: neoculin acidic subunit

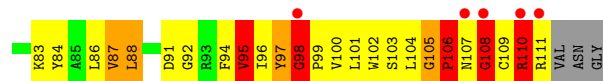
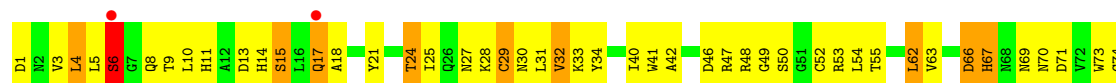


• Molecule 1: neoculin acidic subunit

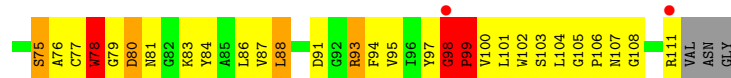




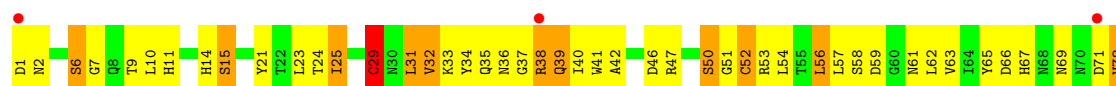
● Molecule 2: Curculin



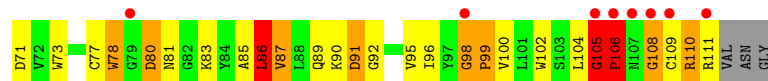
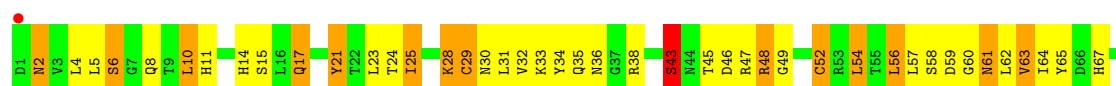
● Molecule 2: Curculin



● Molecule 2: Curculin



● Molecule 2: Curculin



● Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta a-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.01Å 101.09Å 271.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.76 20.00 – 2.76	Depositor EDS
% Data completeness (in resolution range)	92.8 (20.00-2.76) 92.5 (20.00-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.00 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.267 0.246 , 0.268	Depositor DCC
R_{free} test set	3255 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.806	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7112	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: FUL, NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.96	0/873	2.10	22/1190 (1.8%)
1	C	0.97	1/890 (0.1%)	1.63	18/1212 (1.5%)
1	E	1.13	3/873 (0.3%)	1.78	26/1190 (2.2%)
1	G	0.94	1/867 (0.1%)	1.77	15/1182 (1.3%)
2	B	0.99	0/884	1.71	22/1200 (1.8%)
2	D	1.06	0/884	1.87	30/1200 (2.5%)
2	F	0.93	1/873 (0.1%)	1.76	29/1186 (2.4%)
2	H	0.97	0/884	1.71	21/1200 (1.8%)
All	All	1.00	6/7028 (0.1%)	1.80	183/9560 (1.9%)

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	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	103	PRO	CA-C	-9.26	1.39	1.52
1	E	103	PRO	CA-C	-7.67	1.41	1.52
1	E	104	LEU	N-CA	-6.17	1.38	1.46
1	G	102	TRP	N-CA	-5.64	1.38	1.46
2	F	78	TRP	CA-C	-5.43	1.46	1.53
1	E	102	TRP	N-CA	-5.08	1.39	1.45

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ASN	OD1-CG-ND2	-44.77	77.83	122.60
1	G	102	TRP	CA-C-N	-15.06	101.01	119.84
1	G	102	TRP	C-N-CA	-15.06	101.01	119.84
1	E	103	PRO	CA-N-CD	-15.03	90.95	112.00
1	C	103	PRO	CA-N-CD	-13.96	92.46	112.00
2	D	79	GLY	N-CA-C	-13.70	92.16	111.20
2	B	110	ARG	N-CA-C	-13.52	87.25	109.96
2	H	29	CYS	N-CA-C	13.29	128.93	113.38
2	F	36	ASN	CB-CA-C	-12.14	93.40	112.09
2	H	105	GLY	CA-C-N	11.77	134.55	119.84
2	H	105	GLY	C-N-CA	11.77	134.55	119.84
1	A	81	ASN	CB-CG-ND2	11.61	133.82	116.40
1	E	36	HIS	CB-CA-C	-11.22	94.04	111.66
1	G	36	HIS	CB-CA-C	-11.10	95.29	111.95
1	A	36	HIS	CB-CA-C	-10.96	94.19	111.51
2	D	97	TYR	CA-C-N	10.87	138.93	121.87
2	D	97	TYR	C-N-CA	10.87	138.93	121.87
2	F	98	GLY	CA-C-N	-10.50	106.72	119.84
2	F	98	GLY	C-N-CA	-10.50	106.72	119.84
2	D	98	GLY	CA-C-N	-10.31	106.95	119.84
2	D	98	GLY	C-N-CA	-10.31	106.95	119.84
1	G	48	GLN	N-CA-C	-10.19	101.51	112.93
1	E	28	ASN	N-CA-C	-9.88	94.38	109.79
1	E	102	TRP	CB-CA-C	8.89	123.30	109.96
1	G	102	TRP	N-CA-C	8.59	128.80	109.81
2	F	21	TYR	N-CA-C	8.54	123.90	110.32
1	A	102	TRP	CA-C-N	-8.48	109.23	119.84
1	A	102	TRP	C-N-CA	-8.48	109.23	119.84
2	B	98	GLY	CA-C-N	-8.34	111.77	120.03
2	B	98	GLY	C-N-CA	-8.34	111.77	120.03
1	A	32	VAL	N-CA-C	8.33	119.92	107.75
2	B	105	GLY	CA-C-N	8.31	130.22	119.84
2	B	105	GLY	C-N-CA	8.31	130.22	119.84
1	C	40	ILE	CB-CA-C	-8.24	103.39	111.30
2	F	2	ASN	N-CA-C	-8.04	101.37	112.30
2	H	2	ASN	N-CA-C	-8.03	101.97	112.41
1	C	91	ASP	N-CA-C	-8.02	103.39	113.02
1	C	103	PRO	CA-C-N	-7.94	106.37	121.54
1	C	103	PRO	C-N-CA	-7.94	106.37	121.54
2	H	49	GLY	N-CA-C	-7.83	100.68	111.09
2	F	7	GLY	N-CA-C	-7.66	105.57	114.69
2	F	75	SER	N-CA-C	-7.66	103.39	112.89
2	D	99	PRO	CA-N-CD	-7.61	101.34	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	86	LEU	CA-C-N	-7.49	112.34	122.98
2	D	86	LEU	C-N-CA	-7.49	112.34	122.98
2	F	78	TRP	CA-C-N	-7.39	106.92	121.41
2	F	78	TRP	C-N-CA	-7.39	106.92	121.41
2	F	29	CYS	N-CA-C	7.33	127.95	113.29
1	A	16	LEU	N-CA-C	-7.27	100.05	110.59
1	C	16	LEU	N-CA-C	-7.26	99.74	110.48
1	E	28	ASN	CA-C-N	-7.20	112.44	123.17
1	E	28	ASN	C-N-CA	-7.20	112.44	123.17
2	D	97	TYR	O-C-N	7.19	131.40	123.13
2	D	47	ARG	CA-C-N	-7.15	109.55	121.92
2	D	47	ARG	C-N-CA	-7.15	109.55	121.92
1	A	109	CYS	CA-C-N	-7.07	110.86	120.82
1	A	109	CYS	C-N-CA	-7.07	110.86	120.82
2	H	52	CYS	CA-CB-SG	-6.98	98.34	114.40
2	D	108	GLY	N-CA-C	6.96	121.08	112.73
2	D	8	GLN	N-CA-C	6.90	119.62	109.69
2	H	43	SER	N-CA-C	-6.84	104.04	112.38
1	E	101	LEU	CA-C-N	-6.75	110.94	123.55
1	E	101	LEU	C-N-CA	-6.75	110.94	123.55
2	F	77	CYS	CA-C-N	-6.67	110.58	122.32
2	F	77	CYS	C-N-CA	-6.67	110.58	122.32
1	G	59	ASP	N-CA-C	-6.66	104.72	112.92
2	D	29	CYS	CA-C-N	-6.65	113.32	122.30
2	D	29	CYS	C-N-CA	-6.65	113.32	122.30
2	F	92	GLY	CA-C-N	-6.64	112.27	122.09
2	F	92	GLY	C-N-CA	-6.64	112.27	122.09
2	F	97	TYR	CA-C-N	6.62	132.26	121.87
2	F	97	TYR	C-N-CA	6.62	132.26	121.87
1	A	26	GLN	N-CA-C	6.61	119.48	110.55
2	H	106	PRO	N-CA-C	6.59	126.05	112.47
1	A	86	LEU	CA-C-N	-6.58	114.52	123.14
1	A	86	LEU	C-N-CA	-6.58	114.52	123.14
1	C	104	LEU	N-CA-C	-6.57	96.82	110.80
1	G	31	LEU	N-CA-C	-6.56	98.53	108.96
1	A	110	ARG	N-CA-C	-6.51	100.40	110.10
2	B	29	CYS	N-CA-CB	-6.47	107.63	114.10
1	A	89	GLN	N-CA-C	6.39	119.85	110.59
1	C	93	LEU	CA-C-N	-6.38	113.99	122.99
1	C	93	LEU	C-N-CA	-6.38	113.99	122.99
1	E	75	SER	N-CA-C	-6.33	105.05	112.89
2	F	69	ASN	CA-C-N	-6.31	113.30	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	69	ASN	C-N-CA	-6.31	113.30	122.19
2	D	75	SER	N-CA-C	-6.29	104.66	112.90
1	G	32	VAL	N-CA-C	6.29	116.91	108.11
2	B	66	ASP	N-CA-CB	-6.28	101.75	110.29
1	E	49	GLY	N-CA-C	-6.25	103.31	111.37
2	B	62	LEU	CA-C-N	-6.22	113.75	122.71
2	B	62	LEU	C-N-CA	-6.22	113.75	122.71
2	B	24	THR	CA-C-N	-6.22	114.59	122.43
2	B	24	THR	C-N-CA	-6.22	114.59	122.43
2	B	29	CYS	N-CA-C	6.21	122.94	113.51
2	F	32	VAL	N-CA-C	6.17	117.90	108.71
2	B	6	SER	N-CA-C	6.10	118.72	108.23
1	E	104	LEU	N-CA-C	-6.08	95.47	107.69
1	A	36	HIS	N-CA-C	6.06	120.00	112.24
2	D	16	LEU	N-CA-C	-6.05	99.85	109.59
1	A	101	LEU	CA-C-N	-6.05	107.05	121.80
1	A	101	LEU	C-N-CA	-6.05	107.05	121.80
2	H	106	PRO	CA-N-CD	-5.99	103.62	112.00
1	G	15	SER	N-CA-C	5.96	116.42	108.38
2	F	86	LEU	CA-C-N	-5.95	115.34	123.14
2	F	86	LEU	C-N-CA	-5.95	115.34	123.14
1	E	36	HIS	N-CA-C	5.94	119.74	111.90
1	E	6	SER	CA-C-N	-5.88	114.08	123.31
1	E	6	SER	C-N-CA	-5.88	114.08	123.31
2	H	91	ASP	N-CA-C	-5.84	106.24	113.19
1	E	15	SER	N-CA-C	5.83	118.27	109.23
2	B	67	HIS	N-CA-C	-5.81	106.17	113.20
2	H	78	TRP	N-CA-C	5.81	118.24	109.23
2	B	99	PRO	CA-N-CD	-5.81	103.87	112.00
2	B	106	PRO	CA-C-N	-5.80	111.02	120.71
2	B	106	PRO	C-N-CA	-5.80	111.02	120.71
2	B	95	VAL	N-CA-C	5.76	117.64	108.89
2	H	21	TYR	N-CA-C	5.74	119.31	110.42
2	H	95	VAL	N-CA-C	5.71	116.70	108.48
1	A	63	ILE	N-CA-C	5.71	118.16	108.86
1	A	75	SER	N-CA-C	-5.70	106.48	113.50
2	D	2	ASN	N-CA-C	5.69	118.17	110.88
1	G	26	GLN	N-CA-C	5.67	118.73	110.17
1	G	88	LEU	N-CA-C	-5.65	99.91	108.67
2	D	64	ILE	CA-C-N	-5.62	113.82	122.87
2	D	64	ILE	C-N-CA	-5.62	113.82	122.87
2	B	32	VAL	N-CA-C	5.62	115.98	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	6	SER	CA-C-N	-5.62	110.40	121.41
2	D	6	SER	C-N-CA	-5.62	110.40	121.41
1	G	43	SER	N-CA-C	-5.59	105.95	112.89
1	C	2	SER	N-CA-C	-5.58	106.52	113.15
2	F	40	ILE	N-CA-C	5.57	118.55	113.20
2	H	86	LEU	CA-C-N	-5.53	114.74	122.75
2	H	86	LEU	C-N-CA	-5.53	114.74	122.75
2	F	78	TRP	N-CA-C	5.51	115.51	108.24
1	C	26	GLN	N-CA-C	5.49	117.62	110.53
1	E	31	LEU	N-CA-C	-5.41	100.97	109.25
1	C	44	ASP	N-CA-C	-5.39	104.21	111.54
2	D	59	ASP	N-CA-C	-5.38	106.40	113.17
2	F	15	SER	N-CA-C	5.37	116.44	108.60
1	A	49	GLY	N-CA-C	-5.36	103.95	111.09
2	D	21	TYR	N-CA-C	5.35	118.21	109.59
1	G	94	PHE	N-CA-C	-5.34	101.00	109.59
2	D	72	VAL	N-CA-C	5.33	118.58	111.44
1	E	1	ASP	CA-C-N	5.31	129.18	120.63
1	E	1	ASP	C-N-CA	5.31	129.18	120.63
1	C	96	ILE	CA-C-N	-5.30	115.33	123.07
1	C	96	ILE	C-N-CA	-5.30	115.33	123.07
2	H	54	LEU	N-CA-C	5.30	117.54	108.90
1	E	29	CYS	CA-C-N	-5.29	115.15	122.30
1	E	29	CYS	C-N-CA	-5.29	115.15	122.30
1	E	86	LEU	N-CA-C	-5.29	100.68	109.46
2	F	94	PHE	N-CA-C	-5.29	101.08	109.96
2	D	78	TRP	CA-CB-CG	-5.28	103.57	113.60
2	F	37	GLY	CA-C-N	-5.27	113.68	122.64
2	F	37	GLY	C-N-CA	-5.27	113.68	122.64
1	C	43	SER	N-CA-C	-5.27	106.11	112.54
1	C	102	TRP	CB-CA-C	5.23	120.48	110.17
2	F	80	ASP	CB-CA-C	5.23	118.33	109.50
1	A	93	LEU	CA-C-N	-5.22	115.69	123.11
1	A	93	LEU	C-N-CA	-5.22	115.69	123.11
1	C	113	ASN	N-CA-CB	5.22	119.38	110.50
1	C	64	ILE	N-CA-C	-5.21	100.87	108.17
2	H	32	VAL	N-CA-C	5.18	116.05	108.53
1	E	24	THR	N-CA-C	5.17	117.83	109.40
1	E	63	ILE	CA-C-N	-5.17	116.42	122.93
1	E	63	ILE	C-N-CA	-5.17	116.42	122.93
2	H	56	LEU	N-CA-C	-5.16	100.33	108.73
1	G	102	TRP	CA-CB-CG	-5.15	103.81	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	41	TRP	N-CA-C	-5.15	100.49	108.42
2	H	34	TYR	N-CA-C	5.14	117.83	109.24
2	B	97	TYR	CA-C-N	5.12	129.91	121.87
2	B	97	TYR	C-N-CA	5.12	129.91	121.87
2	D	94	PHE	N-CA-C	-5.09	101.11	109.40
2	D	1	ASP	CA-C-N	-5.08	113.53	123.13
2	D	1	ASP	C-N-CA	-5.08	113.53	123.13
1	G	104	LEU	N-CA-C	-5.08	100.45	108.73
1	E	72	VAL	CB-CA-C	-5.07	106.59	111.06
2	H	63	VAL	N-CA-C	5.07	116.91	108.99
1	E	2	SER	N-CA-C	5.06	118.91	112.34
2	H	25	ILE	N-CA-C	-5.04	100.52	108.23
2	F	98	GLY	CA-C-O	-5.03	114.33	121.52
2	B	108	GLY	N-CA-C	5.02	125.08	113.18

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	ASN	Sidechain

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	855	0	811	74	0
1	C	872	0	829	78	0
1	E	855	0	812	62	0
1	G	849	0	806	62	0
2	B	866	0	836	65	0
2	D	866	0	836	69	0
2	F	855	0	823	64	0
2	H	866	0	836	60	0
3	I	49	0	43	0	0
4	A	14	0	12	5	0
5	A	27	0	0	5	0
5	B	18	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	24	0	0	4	0
5	D	24	0	0	2	0
5	E	19	0	0	1	0
5	F	17	0	0	3	0
5	G	15	0	0	0	0
5	H	21	0	0	4	0
All	All	7112	0	6644	489	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 36.

All (489) 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)
4:A:801:NAG:O5	4:A:801:NAG:C1	1.84	1.24
1:E:102:TRP:CD2	1:E:103:PRO:HD2	1.71	1.24
1:C:103:PRO:O	1:C:104:LEU:CB	1.91	1.15
1:C:1:ASP:OD2	5:C:132:HOH:O	1.66	1.13
1:E:102:TRP:CG	1:E:103:PRO:HD2	1.86	1.08
1:C:102:TRP:CD2	1:C:103:PRO:HD2	1.89	1.07
2:F:86:LEU:CD1	2:F:96:ILE:HG13	1.86	1.06
1:C:97:TYR:CE1	2:D:100:VAL:HG22	1.93	1.04
1:E:1:ASP:O	1:E:16:LEU:HD22	1.58	1.04
2:D:11:HIS:HB2	2:D:14:HIS:CE1	1.99	0.95
1:C:31:LEU:HB2	1:C:64:ILE:HD11	1.48	0.95
1:A:102:TRP:O	1:A:108:GLY:O	1.85	0.95
2:D:98:GLY:O	2:D:99:PRO:O	1.85	0.95
1:E:61:ASN:HD21	1:E:78:TRP:HE3	1.09	0.92
2:F:86:LEU:HD13	2:F:96:ILE:HG13	1.52	0.91
2:D:78:TRP:H	2:D:78:TRP:CD1	1.70	0.90
1:E:1:ASP:O	1:E:16:LEU:CD2	2.18	0.90
1:C:1:ASP:OD1	1:C:3:VAL:O	1.90	0.89
2:H:15:SER:HB3	2:H:24:THR:HA	1.56	0.88
1:A:90:GLN:H	1:A:90:GLN:HE21	1.22	0.87
1:C:45:THR:HG21	1:C:72:VAL:HG12	1.56	0.87
1:C:103:PRO:O	1:C:104:LEU:HB2	1.10	0.86
1:G:102:TRP:O	1:G:104:LEU:N	2.08	0.86
2:F:86:LEU:HD12	2:F:96:ILE:HG13	1.54	0.86
2:D:93:ARG:HG3	2:D:93:ARG:HH11	1.40	0.85
1:G:102:TRP:O	1:G:103:PRO:C	2.13	0.85
1:C:84:TYR:OH	1:C:99:PRO:HG3	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:TYR:O	1:G:14:HIS:HB2	1.79	0.83
1:C:41:TRP:CZ2	2:D:104:LEU:HD21	2.13	0.82
2:F:86:LEU:HD13	2:F:96:ILE:CG1	2.08	0.82
1:E:96:ILE:HD12	2:F:102:TRP:HE3	1.44	0.82
1:G:63:ILE:HG12	1:G:71:VAL:HG13	1.61	0.81
1:G:10:LEU:HD21	1:G:15:SER:HA	1.63	0.81
2:F:87:VAL:HG13	2:F:97:TYR:HE1	1.46	0.81
1:E:96:ILE:HD12	2:F:102:TRP:CE3	2.17	0.79
1:C:45:THR:HG22	1:C:45:THR:O	1.80	0.79
1:E:102:TRP:CE2	1:E:103:PRO:HD2	2.18	0.79
1:A:5:LEU:O	1:A:8:GLN:HG3	1.84	0.78
2:H:10:LEU:HD13	2:H:25:ILE:HG22	1.63	0.78
1:A:102:TRP:O	1:A:104:LEU:N	2.17	0.78
2:D:78:TRP:CD1	2:D:78:TRP:N	2.45	0.78
1:G:45:THR:O	1:G:45:THR:HG22	1.83	0.77
1:C:97:TYR:CE1	2:D:100:VAL:CG2	2.67	0.77
1:C:97:TYR:CD1	2:D:100:VAL:HG22	2.19	0.77
2:H:46:ASP:OD1	2:H:47:ARG:N	2.18	0.76
1:G:50:SER:O	1:G:67:ASP:HB2	1.85	0.76
2:D:98:GLY:O	2:D:99:PRO:C	2.27	0.76
2:D:6:SER:OG	2:D:84:TYR:N	2.12	0.76
1:E:61:ASN:ND2	1:E:78:TRP:HE3	1.82	0.75
1:C:102:TRP:CG	1:C:103:PRO:HD2	2.20	0.75
1:E:110:ARG:O	1:E:111:SER:HB3	1.86	0.75
1:G:75:SER:HB2	2:H:102:TRP:CE2	2.22	0.74
2:D:47:ARG:HH21	2:D:72:VAL:HG13	1.52	0.74
1:C:102:TRP:CE3	1:C:103:PRO:HD2	2.21	0.74
1:E:60:GLY:O	5:E:118:HOH:O	2.04	0.73
2:B:97:TYR:O	2:B:98:GLY:O	2.06	0.72
2:D:2:ASN:HB3	2:D:17:GLN:O	1.89	0.72
1:A:81:ASN:OD1	4:A:801:NAG:O5	2.07	0.72
1:A:35:GLN:OE1	2:D:14:HIS:HA	1.89	0.72
2:D:6:SER:HG	2:D:84:TYR:H	1.35	0.72
1:E:102:TRP:CG	1:E:103:PRO:CD	2.70	0.72
2:H:63:VAL:HG22	2:H:64:ILE:N	2.05	0.72
2:F:87:VAL:HG13	2:F:97:TYR:CE1	2.25	0.71
1:G:6:SER:HA	1:G:56:LEU:HD13	1.72	0.71
2:F:33:LYS:HB3	2:F:41:TRP:HB3	1.72	0.71
1:A:103:PRO:HG2	2:B:95:VAL:HG13	1.72	0.70
1:G:2:SER:HB3	1:G:17:THR:O	1.91	0.70
1:C:45:THR:HG21	1:C:72:VAL:CG1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:78:TRP:CD1	1:G:106:LEU:HD22	2.26	0.70
2:D:6:SER:O	2:D:56:LEU:O	2.10	0.70
1:A:70:MET:HG2	5:A:824:HOH:O	1.90	0.70
2:F:79:GLY:O	1:G:106:LEU:HD23	1.91	0.69
1:C:45:THR:CG2	1:C:72:VAL:CG1	2.70	0.69
2:B:28:LYS:O	2:B:29:CYS:HB2	1.90	0.69
2:D:28:LYS:C	2:D:29:CYS:SG	2.74	0.69
1:C:97:TYR:O	1:C:98:GLY:O	2.11	0.69
1:A:102:TRP:HE3	2:B:96:ILE:HD12	1.56	0.69
2:D:11:HIS:HB2	2:D:14:HIS:ND1	2.07	0.69
2:H:102:TRP:HA	2:H:108:GLY:O	1.93	0.69
2:D:8:GLN:O	2:D:55:THR:HG23	1.92	0.68
2:F:10:LEU:HD21	2:F:15:SER:HA	1.76	0.68
2:F:87:VAL:CG1	2:F:97:TYR:CE1	2.77	0.68
1:A:102:TRP:CE3	2:B:96:ILE:HD12	2.29	0.67
2:B:66:ASP:HB3	2:B:70:ASN:H	1.59	0.67
2:H:109:CYS:C	2:H:110:ARG:HD2	2.20	0.67
1:A:48:GLN:O	1:A:48:GLN:HG3	1.94	0.66
2:F:6:SER:HA	2:F:56:LEU:HB3	1.77	0.66
1:A:97:TYR:O	1:A:98:GLY:O	2.14	0.66
1:C:45:THR:CG2	1:C:72:VAL:HG12	2.24	0.66
1:G:47:GLY:C	1:G:49:GLY:H	2.03	0.66
1:C:84:TYR:CE2	1:C:98:GLY:HA2	2.31	0.65
2:D:98:GLY:C	2:D:99:PRO:O	2.39	0.65
1:E:10:LEU:HB3	1:E:54:LEU:HB3	1.78	0.65
1:C:96:ILE:HG13	2:D:102:TRP:HE3	1.60	0.65
1:C:102:TRP:CD2	1:C:103:PRO:CD	2.75	0.65
1:E:31:LEU:HD11	1:E:54:LEU:HD22	1.78	0.65
2:B:32:VAL:HG12	2:B:34:TYR:CE1	2.32	0.64
2:H:48:ARG:O	2:H:48:ARG:HG3	1.97	0.64
1:G:10:LEU:HD23	1:G:25:ILE:HG22	1.78	0.64
1:C:80:ASN:O	1:C:81:ASN:C	2.40	0.64
1:E:102:TRP:HE3	2:F:96:ILE:HD12	1.62	0.64
2:D:10:LEU:HB3	2:D:54:LEU:HB3	1.80	0.64
1:G:97:TYR:O	1:G:98:GLY:O	2.14	0.64
2:B:107:ASN:O	2:B:109:CYS:N	2.31	0.64
2:B:55:THR:O	2:B:62:LEU:HD12	1.97	0.64
1:A:12:ALA:HB1	1:A:27:ASN:HA	1.80	0.63
1:C:84:TYR:CZ	1:C:99:PRO:HG3	2.33	0.63
1:A:82:GLY:HA2	4:A:801:NAG:HN2	1.64	0.63
2:B:62:LEU:O	2:B:74:GLY:HA2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ASN:ND2	1:A:27:ASN:H	1.97	0.63
1:G:9:THR:HG21	1:G:53:ARG:HD2	1.80	0.62
1:E:61:ASN:OD1	1:E:77:CYS:N	2.29	0.62
1:G:28:ASN:O	1:G:47:GLY:N	2.31	0.62
1:G:102:TRP:CG	1:G:103:PRO:N	2.62	0.62
1:G:10:LEU:O	1:G:25:ILE:HG21	2.00	0.62
1:E:61:ASN:OD1	1:E:77:CYS:C	2.42	0.62
1:A:35:GLN:NE2	2:D:15:SER:H	1.97	0.61
2:F:78:TRP:HD1	1:G:106:LEU:HD22	1.65	0.61
2:D:63:VAL:HG12	2:D:64:ILE:N	2.13	0.61
2:H:6:SER:O	2:H:56:LEU:O	2.18	0.61
1:E:61:ASN:OD1	1:E:77:CYS:O	2.18	0.61
1:A:35:GLN:HE22	2:D:15:SER:H	1.48	0.61
2:F:102:TRP:HD1	2:F:109:CYS:HB2	1.66	0.61
2:D:103:SER:HB3	5:D:121:HOH:O	2.00	0.60
2:H:21:TYR:HE2	2:H:90:LYS:O	1.83	0.60
1:C:41:TRP:CZ2	2:D:104:LEU:CD2	2.82	0.60
1:C:106:LEU:O	1:C:108:GLY:N	2.33	0.60
2:F:11:HIS:O	2:F:14:HIS:HB2	2.01	0.60
1:A:63:ILE:HG23	1:A:71:VAL:HG13	1.83	0.60
1:C:100:VAL:CG1	1:C:102:TRP:O	2.50	0.60
1:C:113:ASN:O	1:C:113:ASN:ND2	2.35	0.59
1:G:104:LEU:O	1:G:108:GLY:HA3	2.02	0.59
2:H:63:VAL:HG11	2:H:65:TYR:CZ	2.37	0.59
2:F:87:VAL:CG1	2:F:97:TYR:HE1	2.14	0.59
2:D:28:LYS:O	2:D:29:CYS:SG	2.61	0.59
1:G:66:ASP:HB3	1:G:72:VAL:HG11	1.85	0.59
1:A:90:GLN:H	1:A:90:GLN:NE2	1.98	0.59
1:C:100:VAL:HG12	1:C:102:TRP:O	2.03	0.59
2:F:32:VAL:HG11	2:F:34:TYR:CZ	2.37	0.59
2:F:97:TYR:O	2:F:98:GLY:O	2.21	0.59
1:A:77:CYS:O	5:A:812:HOH:O	2.17	0.58
2:B:6:SER:OG	2:B:84:TYR:N	2.20	0.58
2:D:71:ASP:CG	2:D:71:ASP:O	2.46	0.58
2:H:21:TYR:CE2	2:H:90:LYS:O	2.56	0.58
1:E:28:ASN:HB2	1:E:47:GLY:H	1.68	0.58
2:B:5:LEU:N	2:B:8:GLN:OE1	2.37	0.58
1:E:102:TRP:CD1	1:E:103:PRO:HD2	2.36	0.58
1:E:31:LEU:HB3	1:E:43:SER:HB3	1.86	0.58
1:C:29:CYS:HB2	1:C:49:GLY:O	2.02	0.58
2:D:26:GLN:NE2	2:D:30:ASN:HB3	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:VAL:HG12	1:E:33:LYS:O	2.04	0.58
1:E:110:ARG:O	1:E:111:SER:CB	2.52	0.57
2:H:31:LEU:N	2:H:43:SER:OG	2.32	0.57
2:F:57:LEU:C	2:F:59:ASP:H	2.11	0.57
1:C:84:TYR:HH	1:C:99:PRO:HG3	1.68	0.57
5:C:125:HOH:O	2:D:83:LYS:HB3	2.03	0.57
1:G:75:SER:HB2	2:H:102:TRP:CD2	2.38	0.57
4:A:801:NAG:O5	4:A:801:NAG:C2	2.52	0.57
2:D:93:ARG:HG3	2:D:93:ARG:NH1	2.13	0.57
2:B:15:SER:HB3	2:B:24:THR:OG1	2.05	0.57
1:C:83:THR:HB	1:C:100:VAL:HG23	1.87	0.57
2:D:47:ARG:NH2	2:D:72:VAL:HG13	2.18	0.57
1:G:5:LEU:O	1:G:8:GLN:HG3	2.03	0.57
2:B:25:ILE:HG23	2:B:25:ILE:O	2.05	0.56
2:H:64:ILE:HD12	2:H:73:TRP:HB3	1.87	0.56
1:E:1:ASP:OD1	1:E:1:ASP:C	2.48	0.56
2:F:25:ILE:HA	2:F:31:LEU:HD23	1.87	0.56
1:G:45:THR:O	1:G:45:THR:CG2	2.53	0.56
2:H:11:HIS:O	2:H:14:HIS:HB2	2.05	0.56
1:A:50:SER:O	1:A:51:GLN:HB2	2.03	0.56
2:F:102:TRP:HA	2:F:108:GLY:O	2.05	0.56
1:A:31:LEU:O	1:A:42:ALA:HA	2.05	0.56
2:D:9:THR:HG21	2:D:11:HIS:CE1	2.41	0.56
1:A:27:ASN:H	1:A:27:ASN:HD22	1.53	0.56
2:B:11:HIS:O	2:B:14:HIS:HB2	2.06	0.56
1:C:1:ASP:O	1:C:16:LEU:CD2	2.53	0.56
1:G:41:TRP:CZ2	2:H:104:LEU:HD11	2.40	0.56
1:A:104:LEU:HB2	1:A:108:GLY:C	2.31	0.56
2:H:59:ASP:HB2	2:H:78:TRP:HB2	1.88	0.55
2:H:83:LYS:HB2	2:H:100:VAL:CG2	2.35	0.55
1:G:3:VAL:HG12	1:G:4:LEU:N	2.21	0.55
2:H:28:LYS:HB3	2:H:47:ARG:HA	1.88	0.55
1:G:102:TRP:CD1	1:G:102:TRP:C	2.79	0.55
2:B:30:ASN:ND2	2:B:32:VAL:CG2	2.70	0.55
1:E:1:ASP:O	1:E:16:LEU:HD23	2.06	0.55
2:H:80:ASP:OD1	2:H:80:ASP:N	2.37	0.55
2:D:91:ASP:OD2	2:D:93:ARG:NH1	2.40	0.55
1:E:26:GLN:NE2	1:E:34:TYR:OH	2.40	0.55
2:F:46:ASP:O	2:F:47:ARG:HB2	2.07	0.55
2:F:57:LEU:C	2:F:59:ASP:N	2.65	0.55
2:H:63:VAL:CG2	2:H:64:ILE:N	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:90:LYS:C	2:H:92:GLY:H	2.13	0.55
1:C:26:GLN:NE2	1:C:34:TYR:OH	2.40	0.54
1:G:86:LEU:HG	1:G:86:LEU:O	2.07	0.54
1:A:5:LEU:HD22	2:B:97:TYR:OH	2.07	0.54
1:C:41:TRP:CH2	2:D:104:LEU:HD21	2.41	0.54
1:A:25:ILE:HD13	1:A:54:LEU:HB2	1.89	0.54
1:A:25:ILE:HG23	1:A:25:ILE:O	2.07	0.54
1:A:66:ASP:OD1	1:A:66:ASP:C	2.50	0.54
2:H:28:LYS:HG3	5:H:119:HOH:O	2.08	0.54
2:D:99:PRO:HD2	2:D:111:ARG:NH2	2.23	0.54
1:E:102:TRP:CE2	1:E:103:PRO:CD	2.91	0.54
2:H:100:VAL:HB	5:H:133:HOH:O	2.07	0.54
1:G:110:ARG:HH22	2:H:98:GLY:HA3	1.71	0.54
1:C:106:LEU:C	1:C:108:GLY:H	2.16	0.53
2:F:83:LYS:HB2	2:F:100:VAL:HG23	1.89	0.53
1:C:28:ASN:O	1:C:29:CYS:CB	2.57	0.53
2:F:1:ASP:OD2	5:F:117:HOH:O	2.18	0.53
2:D:63:VAL:CG1	2:D:64:ILE:N	2.71	0.53
2:B:48:ARG:NH1	2:F:73:TRP:HA	2.24	0.53
1:E:9:THR:HG21	1:E:11:TYR:CE1	2.44	0.53
1:G:98:GLY:N	2:H:99:PRO:O	2.36	0.53
1:A:104:LEU:HD12	1:A:110:ARG:N	2.24	0.53
1:E:52:CYS:SG	1:E:66:ASP:HA	2.48	0.53
2:B:101:LEU:HB2	2:B:110:ARG:NH1	2.23	0.53
2:B:86:LEU:HD11	2:B:94:PHE:HD1	1.73	0.53
1:G:23:LEU:HD13	1:G:33:LYS:HG3	1.91	0.53
1:A:104:LEU:HB2	1:A:108:GLY:O	2.10	0.52
2:H:15:SER:CB	2:H:24:THR:HA	2.34	0.52
1:A:11:TYR:O	1:A:14:HIS:HB2	2.09	0.52
1:E:5:LEU:HD23	1:E:85:ALA:HA	1.91	0.52
1:A:58:SER:OG	1:A:81:ASN:ND2	2.42	0.52
1:C:63:ILE:HG23	1:C:71:VAL:HG13	1.91	0.52
2:F:62:LEU:HD13	2:F:86:LEU:HD22	1.91	0.52
2:B:33:LYS:HG2	2:B:40:ILE:CG1	2.40	0.52
1:E:51:GLN:HB2	1:E:67:ASP:HB3	1.90	0.52
1:G:15:SER:HB3	1:G:24:THR:HA	1.92	0.52
1:A:61:ASN:HD21	1:A:76:ASP:H	1.58	0.52
1:C:102:TRP:CG	1:C:103:PRO:CD	2.91	0.52
1:C:35:GLN:O	1:C:36:HIS:HB2	2.10	0.51
1:E:31:LEU:HB2	1:E:64:ILE:HD11	1.91	0.51
1:G:89:GLN:HG2	2:H:5:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:GLN:NE2	2:D:42:ALA:HB2	2.26	0.51
1:C:99:PRO:O	1:C:100:VAL:C	2.52	0.51
1:E:5:LEU:HD13	2:F:97:TYR:OH	2.10	0.51
1:G:102:TRP:HZ2	1:G:107:ASN:ND2	2.06	0.51
1:A:109:CYS:O	1:A:110:ARG:C	2.52	0.51
2:B:104:LEU:O	5:B:126:HOH:O	2.20	0.51
1:C:101:LEU:HD21	2:D:77:CYS:O	2.10	0.51
2:D:47:ARG:CZ	2:D:72:VAL:HG22	2.41	0.51
1:E:25:ILE:O	1:E:25:ILE:HG23	2.11	0.51
1:E:31:LEU:CD1	1:E:54:LEU:HD22	2.41	0.51
1:A:28:ASN:O	1:A:29:CYS:CB	2.59	0.51
1:C:99:PRO:O	1:C:110:ARG:NH2	2.34	0.51
1:A:26:GLN:OE1	1:A:32:VAL:HG21	2.11	0.51
2:B:46:ASP:O	2:B:47:ARG:HB2	2.10	0.51
2:F:23:LEU:HD11	2:F:31:LEU:HD13	1.92	0.51
1:G:23:LEU:HD11	1:G:31:LEU:HD22	1.92	0.50
2:D:31:LEU:HB2	2:D:64:ILE:HD11	1.94	0.50
2:F:9:THR:HG23	2:F:53:ARG:HG3	1.93	0.50
1:A:31:LEU:HB2	1:A:64:ILE:HD11	1.94	0.50
1:A:48:GLN:HG2	1:A:72:VAL:HG13	1.92	0.50
1:A:70:MET:CG	5:A:824:HOH:O	2.56	0.50
2:B:9:THR:N	5:B:124:HOH:O	2.29	0.50
2:F:39:GLN:NE2	2:F:42:ALA:HB2	2.26	0.50
1:E:50:SER:O	1:E:51:GLN:C	2.55	0.50
2:B:9:THR:HG22	2:B:10:LEU:N	2.25	0.50
2:B:30:ASN:HD21	2:B:42:ALA:HB1	1.77	0.50
1:C:97:TYR:HE1	2:D:100:VAL:CG2	2.23	0.50
2:F:31:LEU:O	2:F:42:ALA:HA	2.11	0.50
2:B:29:CYS:SG	2:B:49:GLY:C	2.95	0.50
1:C:1:ASP:CG	1:C:3:VAL:O	2.55	0.50
1:G:3:VAL:HG22	1:G:87:VAL:HG22	1.94	0.50
1:E:68:ASN:O	1:E:69:ASN:C	2.55	0.50
2:B:1:ASP:HA	5:C:134:HOH:O	2.12	0.49
1:E:62:LEU:HB3	1:E:75:SER:HB3	1.92	0.49
1:A:57:ARG:NH2	1:A:65:TYR:OH	2.45	0.49
2:H:10:LEU:HD13	2:H:25:ILE:CG2	2.39	0.49
2:H:31:LEU:H	2:H:43:SER:HG	1.57	0.49
2:B:28:LYS:O	2:B:29:CYS:CB	2.60	0.49
1:A:4:LEU:CD1	1:A:8:GLN:HB2	2.43	0.49
1:A:48:GLN:HG2	1:A:72:VAL:CG1	2.42	0.49
2:H:71:ASP:OD1	2:H:71:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:MET:O	1:E:72:VAL:HG23	2.12	0.49
2:F:91:ASP:OD1	2:F:91:ASP:C	2.55	0.49
1:A:21:TYR:CE1	1:A:35:GLN:CD	2.91	0.48
2:B:83:LYS:HG2	5:B:120:HOH:O	2.13	0.48
2:H:90:LYS:C	2:H:92:GLY:N	2.67	0.48
2:F:35:GLN:NE2	5:F:122:HOH:O	2.44	0.48
2:H:29:CYS:O	2:H:45:THR:OG1	2.27	0.48
2:H:89:GLN:HB2	2:H:91:ASP:OD1	2.14	0.48
2:B:102:TRP:CG	2:B:103:SER:N	2.80	0.48
1:E:102:TRP:CD1	1:E:103:PRO:CD	2.95	0.48
1:E:104:LEU:HB2	1:E:108:GLY:O	2.13	0.48
2:B:87:VAL:HG13	2:B:97:TYR:HE2	1.79	0.48
1:C:62:LEU:O	1:C:74:GLY:HA2	2.13	0.48
2:B:17:GLN:OE1	1:C:36:HIS:CD2	2.66	0.48
2:B:21:TYR:CG	2:B:92:GLY:HA2	2.48	0.48
2:H:58:SER:HB3	2:H:81:ASN:OD1	2.13	0.48
1:A:62:LEU:HB2	1:A:96:ILE:HD11	1.94	0.48
1:C:110:ARG:HD3	1:C:112:LEU:O	2.13	0.48
1:C:113:ASN:OD1	5:C:114:HOH:O	2.19	0.48
2:F:38:ARG:HA	5:F:129:HOH:O	2.13	0.48
1:A:35:GLN:HB2	1:A:40:ILE:CD1	2.44	0.48
2:B:97:TYR:C	2:B:98:GLY:O	2.55	0.48
1:C:1:ASP:O	1:C:16:LEU:HD23	2.14	0.48
1:C:15:SER:HB3	1:C:22:THR:HG23	1.94	0.48
1:G:43:SER:O	1:G:44:ASP:HB2	2.13	0.48
1:G:6:SER:CA	1:G:56:LEU:HD13	2.44	0.48
1:A:63:ILE:HD13	1:A:74:GLY:CA	2.44	0.48
1:C:1:ASP:O	1:C:16:LEU:HD22	2.13	0.48
2:F:11:HIS:HB2	2:F:14:HIS:HD2	1.77	0.48
2:F:86:LEU:HD13	2:F:96:ILE:CD1	2.44	0.48
1:G:3:VAL:CG1	1:G:4:LEU:N	2.77	0.47
2:H:48:ARG:O	2:H:48:ARG:CG	2.59	0.47
2:D:100:VAL:HG12	2:D:101:LEU:N	2.28	0.47
1:G:31:LEU:HB2	1:G:64:ILE:HD11	1.96	0.47
2:H:77:CYS:O	5:H:115:HOH:O	2.20	0.47
2:B:31:LEU:O	2:B:42:ALA:HA	2.14	0.47
2:D:26:GLN:HB2	2:D:30:ASN:O	2.13	0.47
2:F:29:CYS:N	2:F:52:CYS:SG	2.87	0.47
1:E:27:ASN:C	1:E:28:ASN:O	2.51	0.47
1:E:87:VAL:CG1	1:E:97:TYR:HD2	2.28	0.47
1:A:51:GLN:HB2	1:A:67:ASP:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:ASP:OD1	2:H:61:ASN:HB2	2.13	0.47
2:H:98:GLY:O	2:H:99:PRO:O	2.33	0.47
1:E:9:THR:CG2	1:E:11:TYR:CE1	2.98	0.47
2:H:83:LYS:O	2:H:99:PRO:HA	2.15	0.47
2:B:30:ASN:HB2	2:B:46:ASP:CA	2.45	0.47
1:C:1:ASP:OD1	1:C:3:VAL:N	2.46	0.47
1:C:66:ASP:OD1	1:C:70:MET:N	2.45	0.47
2:F:66:ASP:O	2:F:67:HIS:C	2.56	0.47
1:A:104:LEU:HD23	1:A:104:LEU:HA	1.82	0.47
2:F:25:ILE:HG23	2:F:25:ILE:O	2.15	0.47
1:G:6:SER:OG	1:G:84:TYR:N	2.41	0.47
2:B:10:LEU:HD21	2:B:15:SER:HA	1.96	0.46
1:E:109:CYS:SG	1:E:110:ARG:N	2.88	0.46
1:C:38:ARG:HH11	1:C:38:ARG:CG	2.28	0.46
1:E:1:ASP:O	1:E:1:ASP:OD1	2.33	0.46
2:F:72:VAL:O	2:F:72:VAL:CG1	2.63	0.46
1:A:33:LYS:NZ	5:A:802:HOH:O	2.49	0.46
1:A:102:TRP:CE3	1:A:103:PRO:HD3	2.51	0.46
2:B:101:LEU:HD12	2:B:110:ARG:O	2.15	0.46
1:G:47:GLY:C	1:G:49:GLY:N	2.72	0.46
2:D:100:VAL:CG1	2:D:101:LEU:N	2.78	0.46
1:A:107:ASN:OD1	2:F:47:ARG:NH2	2.48	0.46
2:B:54:LEU:HD11	2:B:62:LEU:HG	1.97	0.46
2:B:33:LYS:HG2	2:B:40:ILE:HG12	1.98	0.46
1:A:63:ILE:HD13	1:A:74:GLY:HA2	1.97	0.46
1:C:38:ARG:HH11	1:C:38:ARG:HG3	1.80	0.46
2:H:35:GLN:O	2:H:36:ASN:C	2.57	0.46
1:A:63:ILE:CG2	1:A:71:VAL:HG13	2.46	0.46
2:H:60:GLY:O	5:H:115:HOH:O	2.21	0.46
1:A:25:ILE:CD1	1:A:64:ILE:HD13	2.45	0.46
2:F:9:THR:CG2	2:F:53:ARG:HG3	2.46	0.46
2:F:89:GLN:OE1	2:F:97:TYR:OH	2.25	0.46
2:B:50:SER:O	2:B:67:HIS:HD2	1.98	0.46
2:D:35:GLN:O	2:D:36:ASN:HB2	2.15	0.46
2:D:66:ASP:OD1	2:D:70:ASN:N	2.42	0.46
2:F:86:LEU:CD1	2:F:96:ILE:CG1	2.70	0.46
1:G:107:ASN:OD1	1:G:107:ASN:O	2.34	0.46
2:B:13:ASP:OD1	2:B:27:ASN:N	2.46	0.45
1:E:40:ILE:O	1:E:40:ILE:HG22	2.17	0.45
1:G:32:VAL:HG11	1:G:39:GLN:OE1	2.16	0.45
1:A:2:SER:HB3	1:A:17:THR:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:HH22	2:B:98:GLY:HA2	1.81	0.45
2:H:10:LEU:HB3	2:H:54:LEU:HB3	1.97	0.45
1:C:26:GLN:NE2	1:C:32:VAL:HG21	2.32	0.45
2:F:14:HIS:O	2:F:24:THR:HG23	2.16	0.45
2:H:110:ARG:HD2	2:H:110:ARG:N	2.32	0.45
2:F:11:HIS:HB2	2:F:14:HIS:CD2	2.51	0.45
1:A:63:ILE:HG22	1:A:64:ILE:N	2.30	0.45
1:A:83:THR:O	1:A:99:PRO:HA	2.16	0.45
1:C:84:TYR:HE2	1:C:98:GLY:HA2	1.78	0.45
2:F:10:LEU:HD12	2:F:10:LEU:HA	1.84	0.45
1:A:46:ASP:OD1	1:A:46:ASP:N	2.45	0.45
1:G:66:ASP:OD2	1:G:70:MET:HB2	2.16	0.45
2:B:18:ALA:HB3	2:B:88:LEU:HD13	1.99	0.44
1:C:54:LEU:HD11	1:C:62:LEU:HG	1.99	0.44
1:C:57:ARG:NH2	1:C:59:ASP:OD2	2.47	0.44
1:A:103:PRO:CG	2:B:95:VAL:HG13	2.46	0.44
1:E:11:TYR:O	1:E:14:HIS:HB2	2.18	0.44
1:G:102:TRP:HB3	2:H:96:ILE:HG13	2.00	0.44
2:B:30:ASN:HB2	2:B:46:ASP:HA	1.98	0.44
2:B:103:SER:N	2:B:108:GLY:O	2.51	0.44
2:F:83:LYS:HB2	2:F:100:VAL:CG2	2.47	0.44
2:H:104:LEU:O	2:H:105:GLY:O	2.36	0.44
1:A:63:ILE:CG2	1:A:64:ILE:N	2.81	0.44
2:D:28:LYS:O	2:D:29:CYS:CB	2.65	0.44
1:E:5:LEU:CD2	1:E:85:ALA:HB2	2.48	0.44
1:G:46:ASP:OD1	1:G:46:ASP:N	2.48	0.44
1:A:82:GLY:HA2	4:A:801:NAG:N2	2.32	0.44
2:B:94:PHE:O	2:B:94:PHE:CD1	2.71	0.44
1:C:45:THR:O	1:C:45:THR:CG2	2.53	0.44
1:C:106:LEU:C	1:C:108:GLY:N	2.76	0.44
1:E:26:GLN:O	1:E:28:ASN:O	2.34	0.44
2:F:62:LEU:CD1	2:F:86:LEU:HD22	2.48	0.44
2:F:87:VAL:CG1	2:F:97:TYR:CD1	3.01	0.44
2:H:4:LEU:HB3	2:H:86:LEU:HD23	2.00	0.44
1:C:110:ARG:HH22	2:D:98:GLY:HA2	1.81	0.44
1:G:6:SER:HB2	1:G:83:THR:HG23	2.00	0.44
2:D:54:LEU:HD12	2:D:63:VAL:O	2.17	0.43
2:H:57:LEU:HB3	2:H:58:SER:H	1.64	0.43
1:C:2:SER:HB3	1:C:17:THR:O	2.17	0.43
1:C:70:MET:HE2	1:C:70:MET:HA	1.99	0.43
1:E:102:TRP:HE1	1:E:107:ASN:ND2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:LEU:HA	1:G:94:PHE:HA	1.99	0.43
2:H:86:LEU:HG	2:H:87:VAL:N	2.27	0.43
1:E:5:LEU:O	1:E:6:SER:C	2.61	0.43
1:E:61:ASN:O	1:E:63:ILE:HG12	2.18	0.43
2:F:50:SER:O	2:F:51:GLY:C	2.61	0.43
2:H:61:ASN:HD22	2:H:62:LEU:N	2.16	0.43
1:C:1:ASP:C	1:C:3:VAL:H	2.26	0.43
1:C:99:PRO:HD3	2:D:111:ARG:HH12	1.83	0.43
1:A:4:LEU:HD12	1:A:8:GLN:HB2	1.99	0.43
2:B:3:VAL:HG12	2:B:4:LEU:N	2.33	0.43
2:D:75:SER:O	2:D:76:ALA:C	2.61	0.43
2:H:2:ASN:HB3	2:H:17:GLN:O	2.18	0.43
2:B:70:ASN:ND2	2:F:71:ASP:OD2	2.50	0.43
2:D:23:LEU:HD12	2:D:32:VAL:O	2.19	0.43
2:D:57:LEU:HB3	5:D:130:HOH:O	2.19	0.43
1:E:102:TRP:CD2	1:E:103:PRO:CD	2.67	0.43
2:D:88:LEU:C	2:D:88:LEU:CD2	2.92	0.43
1:E:61:ASN:ND2	1:E:78:TRP:CE3	2.73	0.43
1:C:5:LEU:HB2	1:C:8:GLN:CD	2.43	0.43
2:F:10:LEU:O	2:F:53:ARG:HB2	2.19	0.43
1:A:52:CYS:SG	1:A:66:ASP:HA	2.60	0.42
1:A:100:VAL:HG22	2:B:97:TYR:CE1	2.54	0.42
2:B:48:ARG:CZ	2:F:73:TRP:HA	2.49	0.42
1:C:23:LEU:HD12	1:C:32:VAL:O	2.19	0.42
1:C:63:ILE:HG22	1:C:64:ILE:N	2.34	0.42
1:G:87:VAL:O	1:G:94:PHE:HA	2.19	0.42
1:G:102:TRP:O	1:G:104:LEU:HG	2.19	0.42
1:A:110:ARG:HH22	2:B:98:GLY:CA	2.32	0.42
2:D:59:ASP:OD1	2:D:61:ASN:HB2	2.20	0.42
2:H:33:LYS:NZ	2:H:92:GLY:O	2.44	0.42
1:G:100:VAL:CG1	1:G:104:LEU:CD2	2.98	0.42
1:C:83:THR:HB	1:C:100:VAL:CG2	2.50	0.42
1:C:110:ARG:CD	1:C:112:LEU:O	2.68	0.42
2:D:4:LEU:HD12	2:D:8:GLN:HB2	2.00	0.42
2:D:55:THR:HG22	2:D:56:LEU:N	2.35	0.42
1:E:52:CYS:HA	1:E:65:TYR:O	2.19	0.42
2:H:104:LEU:HD23	2:H:104:LEU:HA	1.82	0.42
2:B:71:ASP:OD1	2:B:71:ASP:O	2.37	0.42
1:C:41:TRP:CD2	2:D:104:LEU:HD11	2.54	0.42
1:G:66:ASP:OD1	1:G:68:ASN:N	2.45	0.42
1:A:5:LEU:O	1:A:6:SER:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ILE:O	1:A:40:ILE:CG2	2.67	0.42
2:B:91:ASP:OD1	2:B:91:ASP:C	2.62	0.42
2:D:80:ASP:OD1	2:D:81:ASN:N	2.52	0.42
2:F:33:LYS:CB	2:F:41:TRP:HB3	2.44	0.42
1:E:89:GLN:C	1:E:91:ASP:H	2.28	0.42
1:G:110:ARG:HH22	2:H:98:GLY:CA	2.32	0.42
2:B:87:VAL:CG1	2:B:97:TYR:CE2	3.03	0.41
1:G:66:ASP:OD1	1:G:66:ASP:C	2.63	0.41
1:G:100:VAL:HG11	1:G:104:LEU:HD23	2.02	0.41
1:E:95:VAL:HG13	2:F:103:SER:HB3	2.02	0.41
2:H:52:CYS:HA	2:H:65:TYR:O	2.21	0.41
2:B:53:ARG:NH1	2:B:69:ASN:OD1	2.53	0.41
2:D:26:GLN:HE21	2:D:30:ASN:HB3	1.84	0.41
1:G:70:MET:O	1:G:72:VAL:HG13	2.20	0.41
2:B:28:LYS:HB2	2:B:28:LYS:HE2	1.80	0.41
2:B:71:ASP:O	2:B:71:ASP:CG	2.62	0.41
1:C:100:VAL:HG13	2:D:95:VAL:CG1	2.50	0.41
2:D:88:LEU:C	2:D:88:LEU:HD22	2.46	0.41
2:D:102:TRP:CG	2:D:103:SER:N	2.86	0.41
1:G:97:TYR:CD2	2:H:85:ALA:HB2	2.55	0.41
2:D:11:HIS:O	2:D:12:ALA:C	2.64	0.41
2:B:41:TRP:CD2	2:B:42:ALA:N	2.89	0.41
1:C:56:LEU:HA	1:C:62:LEU:HD12	2.03	0.41
1:A:6:SER:OG	1:A:84:TYR:N	2.42	0.41
1:A:45:THR:O	1:A:48:GLN:HB3	2.21	0.41
2:B:9:THR:CG2	2:B:10:LEU:N	2.83	0.41
1:C:54:LEU:HD11	1:C:62:LEU:CD2	2.50	0.41
1:E:26:GLN:HB2	1:E:28:ASN:OD1	2.21	0.41
1:E:53:ARG:HH11	1:E:53:ARG:HD2	1.74	0.41
1:E:80:ASN:HD22	1:E:80:ASN:HA	1.62	0.41
1:G:63:ILE:HG21	1:G:65:TYR:CZ	2.56	0.41
2:H:15:SER:HB2	2:H:23:LEU:O	2.20	0.41
1:E:6:SER:N	1:E:56:LEU:HD23	2.36	0.41
1:A:86:LEU:HB2	1:A:96:ILE:HG12	2.03	0.40
2:F:57:LEU:O	2:F:59:ASP:N	2.53	0.40
1:G:100:VAL:HG12	1:G:104:LEU:HD21	2.04	0.40
1:A:110:ARG:O	1:A:111:SER:O	2.37	0.40
2:B:33:LYS:HD2	2:B:40:ILE:HD11	2.03	0.40
2:D:105:GLY:O	2:D:106:PRO:C	2.63	0.40
2:F:63:VAL:HG11	2:F:65:TYR:CZ	2.56	0.40
2:H:61:ASN:OD1	2:H:78:TRP:HE3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:TRP:CG	2:B:74:GLY:N	2.90	0.40
1:C:54:LEU:HD21	1:C:62:LEU:HD21	2.04	0.40
1:A:30:ASN:ND2	5:A:805:HOH:O	2.16	0.40
2:B:105:GLY:HA2	2:B:106:PRO:HD2	1.79	0.40
2:F:54:LEU:HD12	2:F:54:LEU:HA	1.84	0.40
2:H:10:LEU:CB	2:H:54:LEU:HB3	2.51	0.40
1:A:62:LEU:O	1:A:74:GLY:HA2	2.20	0.40
1:C:96:ILE:HG13	2:D:102:TRP:CE3	2.49	0.40
2:D:47:ARG:HE	2:D:72:VAL:HG13	1.86	0.40
2:F:10:LEU:HB3	2:F:54:LEU:HB3	2.04	0.40
1:G:54:LEU:HG	1:G:62:LEU:HD11	2.03	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	109/113 (96%)	97 (89%)	10 (9%)	2 (2%)	6	13
1	C	111/113 (98%)	99 (89%)	7 (6%)	5 (4%)	2	2
1	E	109/113 (96%)	88 (81%)	13 (12%)	8 (7%)	1	1
1	G	108/113 (96%)	97 (90%)	7 (6%)	4 (4%)	2	4
2	B	109/114 (96%)	98 (90%)	8 (7%)	3 (3%)	4	6
2	D	109/114 (96%)	96 (88%)	11 (10%)	2 (2%)	6	13
2	F	108/114 (95%)	92 (85%)	15 (14%)	1 (1%)	14	28
2	H	109/114 (96%)	94 (86%)	10 (9%)	5 (5%)	2	2
All	All	872/908 (96%)	761 (87%)	81 (9%)	30 (3%)	3	5

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	GLY
2	B	98	GLY
2	B	106	PRO
2	B	108	GLY
1	C	98	GLY
1	C	103	PRO
1	C	107	ASN
2	D	98	GLY
1	E	69	ASN
1	E	98	GLY
1	E	103	PRO
2	F	98	GLY
1	G	98	GLY
1	G	102	TRP
2	H	98	GLY
2	H	106	PRO
2	H	108	GLY
1	C	29	CYS
1	C	100	VAL
1	E	26	GLN
1	G	12	ALA
2	D	99	PRO
1	E	51	GLN
1	E	107	ASN
1	E	110	ARG
2	H	99	PRO
1	G	103	PRO
2	H	105	GLY
1	A	102	TRP
1	E	90	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	94/96 (98%)	79 (84%)	15 (16%)	2 4
1	C	96/96 (100%)	84 (88%)	12 (12%)	4 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	94/96 (98%)	79 (84%)	15 (16%)	2	4
1	G	93/96 (97%)	83 (89%)	10 (11%)	6	12
2	B	92/94 (98%)	79 (86%)	13 (14%)	3	6
2	D	92/94 (98%)	78 (85%)	14 (15%)	3	4
2	F	91/94 (97%)	75 (82%)	16 (18%)	2	3
2	H	92/94 (98%)	75 (82%)	17 (18%)	1	3
All	All	744/760 (98%)	632 (85%)	112 (15%)	3	4

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	15	SER
1	A	25	ILE
1	A	27	ASN
1	A	29	CYS
1	A	40	ILE
1	A	46	ASP
1	A	57	ARG
1	A	64	ILE
1	A	70	MET
1	A	86	LEU
1	A	87	VAL
1	A	90	GLN
1	A	110	ARG
1	A	111	SER
2	B	4	LEU
2	B	6	SER
2	B	15	SER
2	B	17	GLN
2	B	52	CYS
2	B	63	VAL
2	B	87	VAL
2	B	88	LEU
2	B	95	VAL
2	B	100	VAL
2	B	106	PRO
2	B	110	ARG
2	B	111	ARG
1	C	17	THR

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Mol	Chain	Res	Type
1	C	25	ILE
1	C	31	LEU
1	C	32	VAL
1	C	38	ARG
1	C	48	GLN
1	C	58	SER
1	C	75	SER
1	C	87	VAL
1	C	96	ILE
1	C	103	PRO
1	C	111	SER
2	D	25	ILE
2	D	28	LYS
2	D	29	CYS
2	D	38	ARG
2	D	48	ARG
2	D	61	ASN
2	D	64	ILE
2	D	72	VAL
2	D	78	TRP
2	D	80	ASP
2	D	87	VAL
2	D	88	LEU
2	D	93	ARG
2	D	107	ASN
1	E	2	SER
1	E	4	LEU
1	E	6	SER
1	E	9	THR
1	E	15	SER
1	E	48	GLN
1	E	53	ARG
1	E	58	SER
1	E	70	MET
1	E	80	ASN
1	E	87	VAL
1	E	95	VAL
1	E	100	VAL
1	E	103	PRO
1	E	104	LEU
2	F	6	SER
2	F	25	ILE

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Mol	Chain	Res	Type
2	F	29	CYS
2	F	31	LEU
2	F	38	ARG
2	F	39	GLN
2	F	50	SER
2	F	52	CYS
2	F	56	LEU
2	F	58	SER
2	F	61	ASN
2	F	72	VAL
2	F	81	ASN
2	F	87	VAL
2	F	93	ARG
2	F	110	ARG
1	G	8	GLN
1	G	10	LEU
1	G	25	ILE
1	G	31	LEU
1	G	39	GLN
1	G	40	ILE
1	G	56	LEU
1	G	58	SER
1	G	63	ILE
1	G	86	LEU
2	H	6	SER
2	H	8	GLN
2	H	10	LEU
2	H	17	GLN
2	H	28	LYS
2	H	30	ASN
2	H	38	ARG
2	H	43	SER
2	H	48	ARG
2	H	61	ASN
2	H	67	HIS
2	H	80	ASP
2	H	86	LEU
2	H	87	VAL
2	H	106	PRO
2	H	110	ARG
2	H	111	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	27	ASN
1	A	36	HIS
1	A	61	ASN
1	A	89	GLN
2	B	26	GLN
2	B	67	HIS
2	B	68	ASN
1	C	36	HIS
1	C	90	GLN
1	C	113	ASN
2	D	11	HIS
2	D	26	GLN
2	D	39	GLN
2	D	81	ASN
1	E	14	HIS
1	E	26	GLN
1	E	27	ASN
1	E	35	GLN
1	E	48	GLN
1	E	68	ASN
1	E	80	ASN
1	E	107	ASN
2	F	2	ASN
2	F	14	HIS
2	F	35	GLN
2	F	61	ASN
2	F	67	HIS
2	F	70	ASN
2	F	81	ASN
1	G	27	ASN
1	G	80	ASN
1	G	90	GLN
1	G	107	ASN
2	H	30	ASN
2	H	61	ASN
2	H	68	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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$
3	NAG	I	1	1,3	14,14,15	0.85	0	17,19,21	1.33	2 (11%)
3	NAG	I	2	3	14,14,15	0.54	0	17,19,21	0.65	0
3	BMA	I	3	3	11,11,12	0.53	0	15,15,17	0.30	0
3	FUL	I	4	3	10,10,11	0.54	0	14,14,16	0.67	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	BMA	I	3	3	-	2/2/19/22	0/1/1/1
3	FUL	I	4	3	-	-	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	NAG	C1-O5-C5	-2.90	108.29	112.19
3	I	1	NAG	O5-C1-C2	-2.61	107.25	111.29
3	I	4	FUL	C1-C2-C3	2.03	112.59	109.64

There are no chirality outliers.

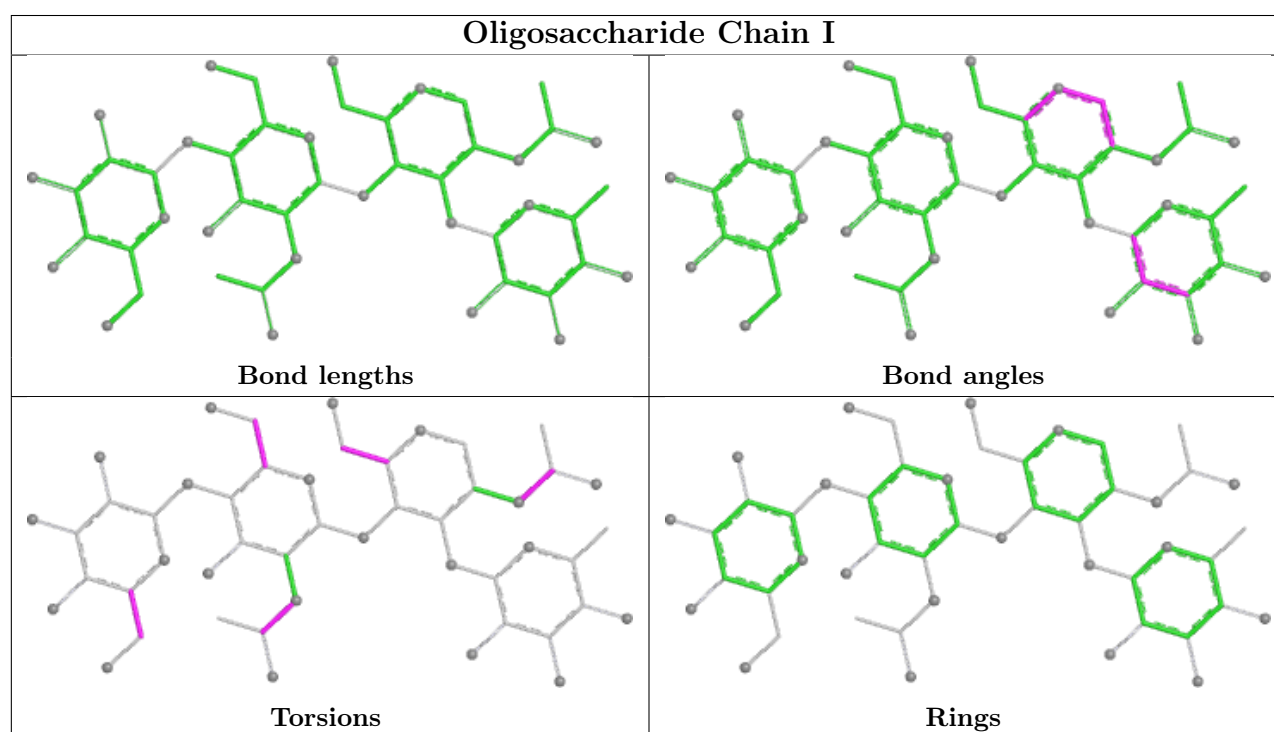
All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	I	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
3	I	3	BMA	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

1 ligand is 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
4	NAG	A	801	1	14,14,15	7.67	5 (35%)	17,19,21	5.06	3 (17%)

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
4	NAG	A	801	1	-	5/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	NAG	O5-C1	24.44	1.84	1.43
4	A	801	NAG	C1-C2	13.53	1.70	1.52
4	A	801	NAG	O5-C5	5.09	1.53	1.43
4	A	801	NAG	C3-C2	3.10	1.59	1.52
4	A	801	NAG	C2-N2	-2.05	1.42	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	NAG	C1-O5-C5	15.20	132.56	112.19
4	A	801	NAG	O5-C1-C2	-13.43	90.52	111.29
4	A	801	NAG	O5-C5-C6	-3.23	101.38	107.66

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	NAG	C3-C2-N2-C7
4	A	801	NAG	C8-C7-N2-C2
4	A	801	NAG	O7-C7-N2-C2
4	A	801	NAG	O5-C5-C6-O6
4	A	801	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	NAG	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	111/113 (98%)	0.24	4 (3%)	46	44	10, 25, 43, 56	0
1	C	113/113 (100%)	0.44	9 (7%)	18	18	9, 26, 47, 58	0
1	E	111/113 (98%)	0.66	9 (8%)	18	18	19, 34, 56, 63	0
1	G	110/113 (97%)	0.47	7 (6%)	25	25	20, 35, 55, 61	0
2	B	111/114 (97%)	0.10	7 (6%)	26	26	10, 23, 43, 72	0
2	D	111/114 (97%)	0.11	2 (1%)	67	65	10, 22, 39, 52	0
2	F	110/114 (96%)	0.30	8 (7%)	21	21	18, 29, 51, 60	0
2	H	111/114 (97%)	0.56	9 (8%)	18	18	22, 39, 57, 79	1 (0%)
All	All	888/908 (97%)	0.36	55 (6%)	26	26	9, 29, 53, 79	1 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	112	LEU	8.3
2	F	79	GLY	8.2
1	C	113	ASN	6.0
2	B	111	ARG	5.2
2	H	79	GLY	4.7
1	C	79	GLY	4.6
1	E	1	ASP	4.6
2	B	98	GLY	4.5
1	E	61	ASN	4.5
2	F	98	GLY	4.5
2	H	1	ASP	4.5
1	G	79	GLY	4.1
2	H	111	ARG	3.9
2	H	98	GLY	3.9
2	F	78	TRP	3.9
2	H	106	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	110	ARG	3.7
2	F	80	ASP	3.6
1	E	103	PRO	3.6
1	C	70	MET	3.3
1	G	48	GLN	3.3
2	H	108	GLY	3.3
1	E	51	GLN	3.2
1	C	99	PRO	3.0
2	B	6	SER	3.0
2	F	1	ASP	2.9
1	A	98	GLY	2.9
1	C	98	GLY	2.9
1	A	111	SER	2.8
2	H	109	CYS	2.8
1	G	106	LEU	2.7
2	D	98	GLY	2.7
1	E	111	SER	2.7
1	E	98	GLY	2.7
2	H	105	GLY	2.6
1	C	107	ASN	2.6
1	G	102	TRP	2.5
2	B	108	GLY	2.5
1	G	45	THR	2.4
2	B	107	ASN	2.4
2	F	71	ASP	2.4
1	E	60	GLY	2.4
1	A	35	GLN	2.4
1	A	81	ASN	2.4
1	E	106	LEU	2.4
1	G	47	GLY	2.4
2	F	110	ARG	2.4
1	G	104	LEU	2.3
2	H	107	ASN	2.2
2	D	111	ARG	2.2
1	E	67	ASP	2.1
1	C	1	ASP	2.1
2	B	17	GLN	2.1
1	C	106	LEU	2.1
2	F	38	ARG	2.0

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

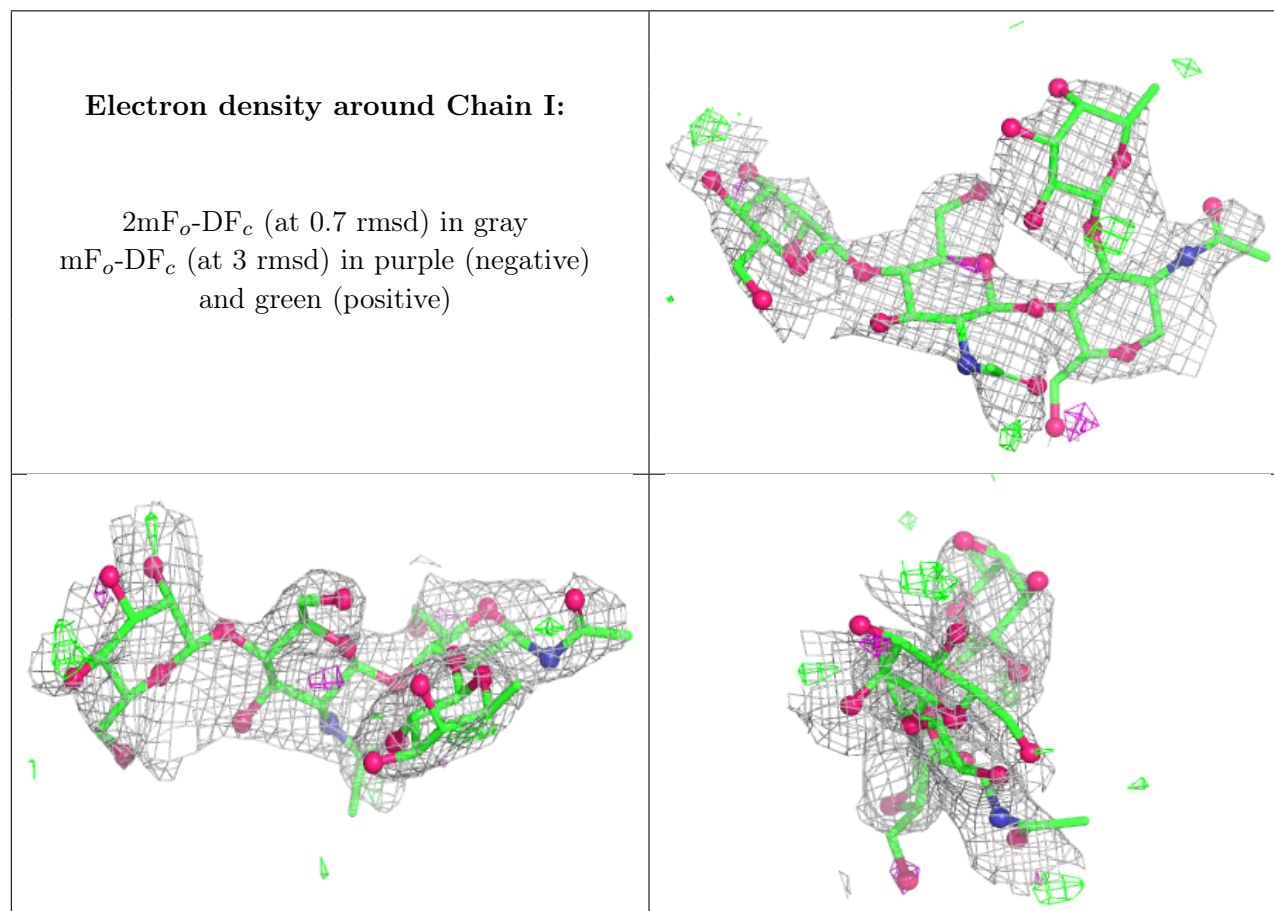
There are no non-standard protein/DNA/RNA residues in this entry.

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
3	BMA	I	3	11/12	0.47	0.24	83,85,86,87	0
3	NAG	I	2	14/15	0.65	0.24	75,79,81,83	0
3	NAG	I	1	14/15	0.66	0.21	72,75,78,79	0
3	FUL	I	4	10/11	0.75	0.18	80,83,83,84	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.



6.4 Ligands

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
4	NAG	A	801	14/15	0.42	0.25	73,79,81,84	0

6.5 Other polymers

There are no such residues in this entry.