Full wwPDB X-ray Structure Validation Report (i)

Oct 28, 2024 – 11:27 am GMT

PDB ID	:	4BSU
Title	:	Structure of the ectodomain of LGR5 in complex with R-spondin-1 (Fu1Fu2) in C2 crystal form
Authors	:	Peng, W.C.; de Lau, W.; Forneris, F.; Granneman, J.C.M.; Huch, M.; Clevers, H.; Gros, P.
Deposited on	:	2013-06-11
Resolution	:	3.20 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:

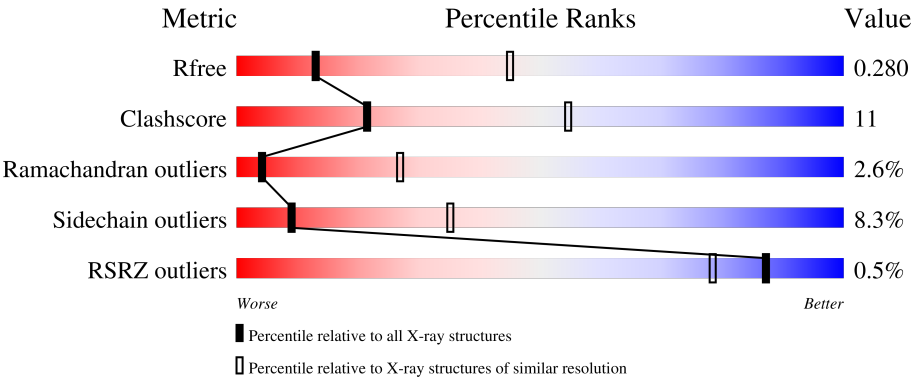
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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	539	64% 21% • 12%
1	B	539	59% 24% • 13%
1	E	539	60% 21% • 14%
1	F	539	58% 23% 5% 14%
2	C	126	59% 17% 6% • 18%

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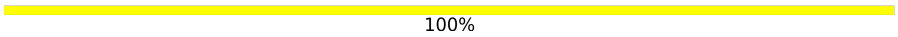
Mol	Chain	Length	Quality of chain
2	D	126	
2	G	126	
2	H	126	
3	I	2	
4	J	3	
4	K	3	
4	L	3	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17955 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 LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	118	0	0
			3725	2377	639	692	17			
1	B	471	Total	C	N	O	S	107	0	0
			3698	2359	633	689	17			
1	E	462	Total	C	N	O	S	0	0	0
			3616	2303	622	674	17			
1	F	463	Total	C	N	O	S	0	0	0
			3630	2313	627	673	17			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	HIS	-	expression tag	UNP O75473
A	9	HIS	-	expression tag	UNP O75473
A	10	HIS	-	expression tag	UNP O75473
A	11	HIS	-	expression tag	UNP O75473
A	12	HIS	-	expression tag	UNP O75473
A	13	HIS	-	expression tag	UNP O75473
A	14	GLU	-	expression tag	UNP O75473
A	15	ASN	-	expression tag	UNP O75473
A	16	LEU	-	expression tag	UNP O75473
A	17	TYR	-	expression tag	UNP O75473
A	18	PHE	-	expression tag	UNP O75473
A	19	GLN	-	expression tag	UNP O75473
A	20	GLY	-	expression tag	UNP O75473
A	21	SER	-	expression tag	UNP O75473
A	544	ALA	-	expression tag	UNP O75473
A	545	ALA	-	expression tag	UNP O75473
A	546	ALA	-	expression tag	UNP O75473
B	8	HIS	-	expression tag	UNP O75473
B	9	HIS	-	expression tag	UNP O75473
B	10	HIS	-	expression tag	UNP O75473

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Chain	Residue	Modelled	Actual	Comment	Reference
B	11	HIS	-	expression tag	UNP O75473
B	12	HIS	-	expression tag	UNP O75473
B	13	HIS	-	expression tag	UNP O75473
B	14	GLU	-	expression tag	UNP O75473
B	15	ASN	-	expression tag	UNP O75473
B	16	LEU	-	expression tag	UNP O75473
B	17	TYR	-	expression tag	UNP O75473
B	18	PHE	-	expression tag	UNP O75473
B	19	GLN	-	expression tag	UNP O75473
B	20	GLY	-	expression tag	UNP O75473
B	21	SER	-	expression tag	UNP O75473
B	544	ALA	-	expression tag	UNP O75473
B	545	ALA	-	expression tag	UNP O75473
B	546	ALA	-	expression tag	UNP O75473
E	8	HIS	-	expression tag	UNP O75473
E	9	HIS	-	expression tag	UNP O75473
E	10	HIS	-	expression tag	UNP O75473
E	11	HIS	-	expression tag	UNP O75473
E	12	HIS	-	expression tag	UNP O75473
E	13	HIS	-	expression tag	UNP O75473
E	14	GLU	-	expression tag	UNP O75473
E	15	ASN	-	expression tag	UNP O75473
E	16	LEU	-	expression tag	UNP O75473
E	17	TYR	-	expression tag	UNP O75473
E	18	PHE	-	expression tag	UNP O75473
E	19	GLN	-	expression tag	UNP O75473
E	20	GLY	-	expression tag	UNP O75473
E	21	SER	-	expression tag	UNP O75473
E	544	ALA	-	expression tag	UNP O75473
E	545	ALA	-	expression tag	UNP O75473
E	546	ALA	-	expression tag	UNP O75473
F	8	HIS	-	expression tag	UNP O75473
F	9	HIS	-	expression tag	UNP O75473
F	10	HIS	-	expression tag	UNP O75473
F	11	HIS	-	expression tag	UNP O75473
F	12	HIS	-	expression tag	UNP O75473
F	13	HIS	-	expression tag	UNP O75473
F	14	GLU	-	expression tag	UNP O75473
F	15	ASN	-	expression tag	UNP O75473
F	16	LEU	-	expression tag	UNP O75473
F	17	TYR	-	expression tag	UNP O75473
F	18	PHE	-	expression tag	UNP O75473

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Chain	Residue	Modelled	Actual	Comment	Reference
F	19	GLN	-	expression tag	UNP O75473
F	20	GLY	-	expression tag	UNP O75473
F	21	SER	-	expression tag	UNP O75473
F	544	ALA	-	expression tag	UNP O75473
F	545	ALA	-	expression tag	UNP O75473
F	546	ALA	-	expression tag	UNP O75473

- Molecule 2 is a protein called R-SPONDIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	103	Total	C	N	O	S	0	0	0
			778	480	137	143	18			
2	D	104	Total	C	N	O	S	0	0	0
			784	483	138	145	18			
2	G	103	Total	C	N	O	S	0	0	0
			772	477	134	143	18			
2	H	104	Total	C	N	O	S	0	0	0
			779	480	137	144	18			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	29	GLY	-	expression tag	UNP Q2MKA7
C	30	SER	-	expression tag	UNP Q2MKA7
C	147	ALA	-	expression tag	UNP Q2MKA7
C	148	ALA	-	expression tag	UNP Q2MKA7
C	149	HIS	-	expression tag	UNP Q2MKA7
C	150	HIS	-	expression tag	UNP Q2MKA7
C	151	HIS	-	expression tag	UNP Q2MKA7
C	152	HIS	-	expression tag	UNP Q2MKA7
C	153	HIS	-	expression tag	UNP Q2MKA7
C	154	HIS	-	expression tag	UNP Q2MKA7
D	29	GLY	-	expression tag	UNP Q2MKA7
D	30	SER	-	expression tag	UNP Q2MKA7
D	147	ALA	-	expression tag	UNP Q2MKA7
D	148	ALA	-	expression tag	UNP Q2MKA7
D	149	HIS	-	expression tag	UNP Q2MKA7
D	150	HIS	-	expression tag	UNP Q2MKA7
D	151	HIS	-	expression tag	UNP Q2MKA7
D	152	HIS	-	expression tag	UNP Q2MKA7
D	153	HIS	-	expression tag	UNP Q2MKA7
D	154	HIS	-	expression tag	UNP Q2MKA7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	29	GLY	-	expression tag	UNP Q2MKA7
G	30	SER	-	expression tag	UNP Q2MKA7
G	147	ALA	-	expression tag	UNP Q2MKA7
G	148	ALA	-	expression tag	UNP Q2MKA7
G	149	HIS	-	expression tag	UNP Q2MKA7
G	150	HIS	-	expression tag	UNP Q2MKA7
G	151	HIS	-	expression tag	UNP Q2MKA7
G	152	HIS	-	expression tag	UNP Q2MKA7
G	153	HIS	-	expression tag	UNP Q2MKA7
G	154	HIS	-	expression tag	UNP Q2MKA7
H	29	GLY	-	expression tag	UNP Q2MKA7
H	30	SER	-	expression tag	UNP Q2MKA7
H	147	ALA	-	expression tag	UNP Q2MKA7
H	148	ALA	-	expression tag	UNP Q2MKA7
H	149	HIS	-	expression tag	UNP Q2MKA7
H	150	HIS	-	expression tag	UNP Q2MKA7
H	151	HIS	-	expression tag	UNP Q2MKA7
H	152	HIS	-	expression tag	UNP Q2MKA7
H	153	HIS	-	expression tag	UNP Q2MKA7
H	154	HIS	-	expression tag	UNP Q2MKA7

- Molecule 3 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			
3	I	2	28	16	2	10	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	J	3	39	22	2	15	0	0	0

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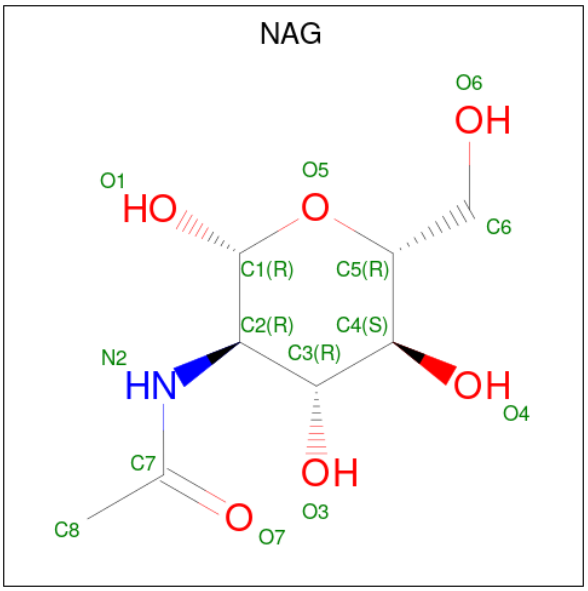
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	K	3	Total C N O 39 22 2 15	0	0	0
4	L	3	Total C N O 39 22 2 15	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



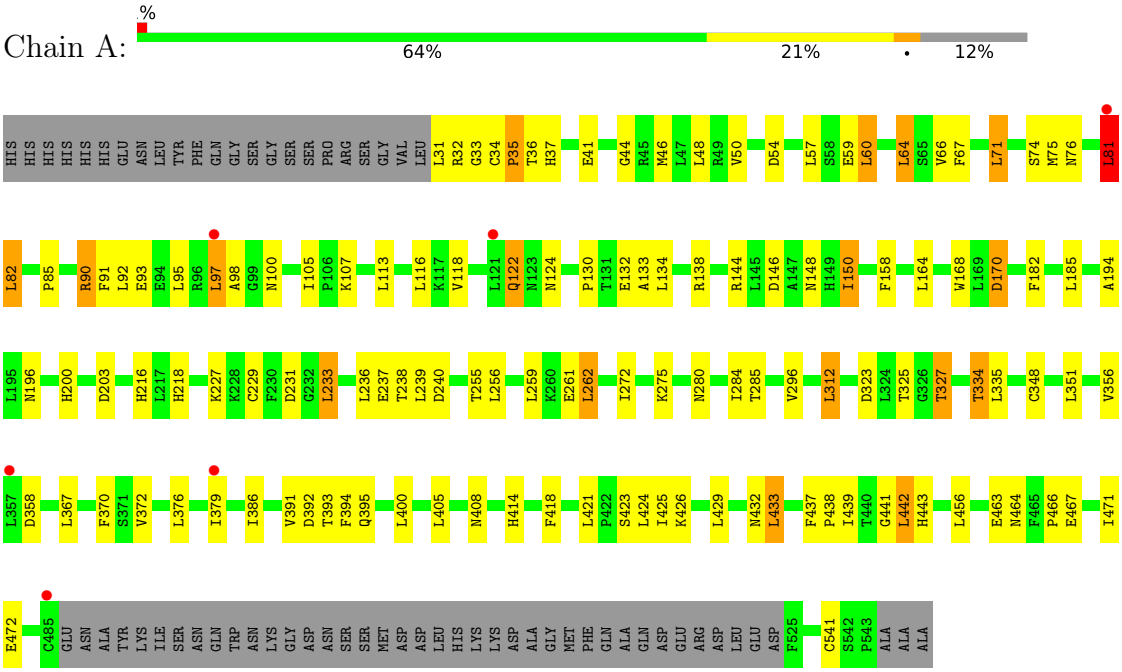
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 14 8 1 5	0	0
5	F	1	Total C N O 14 8 1 5	0	0

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.

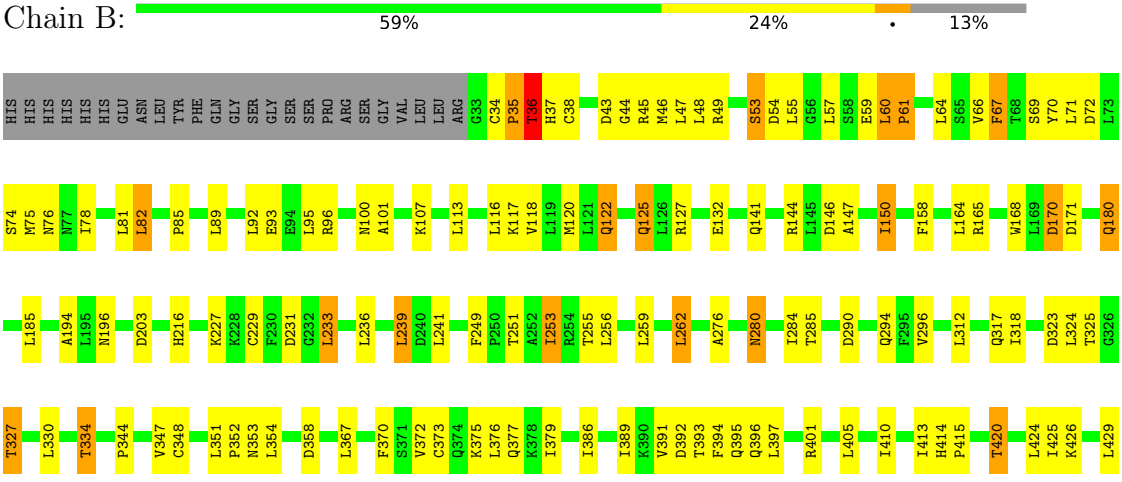
• Molecule 1: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR 5

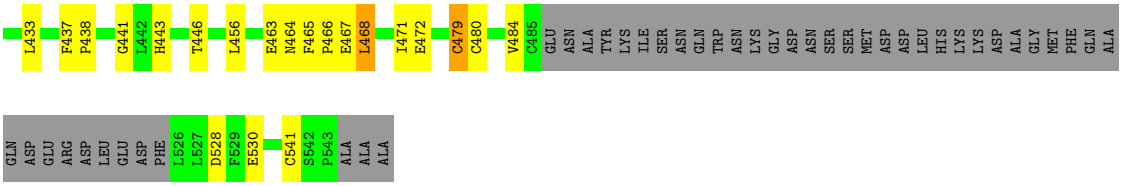
Chain A:



• Molecule 1: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR 5

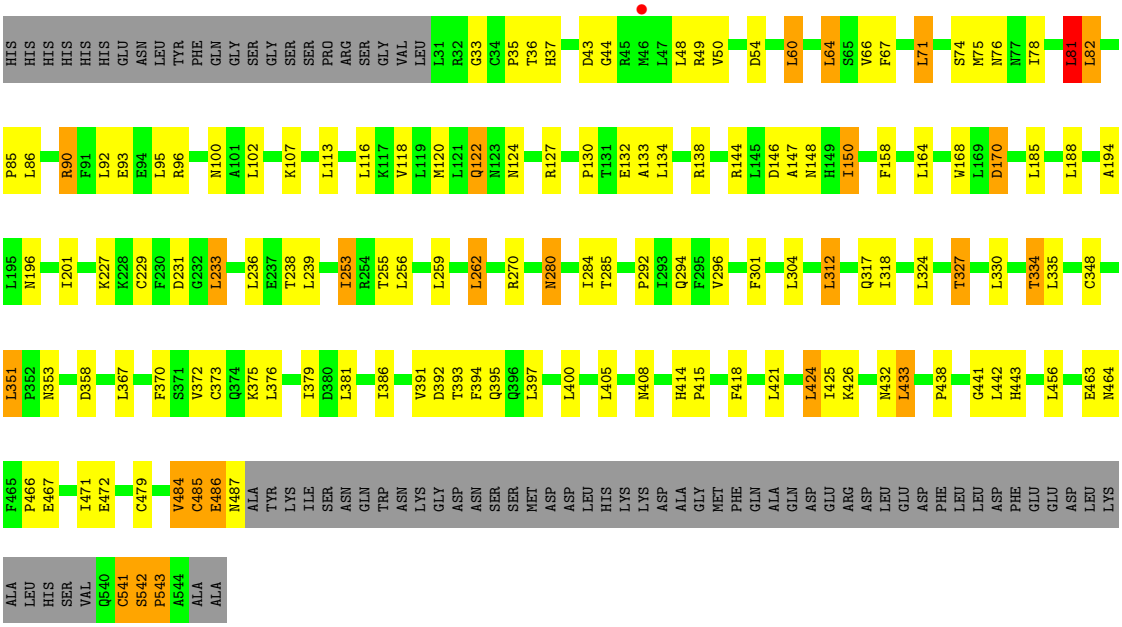
Chain B:





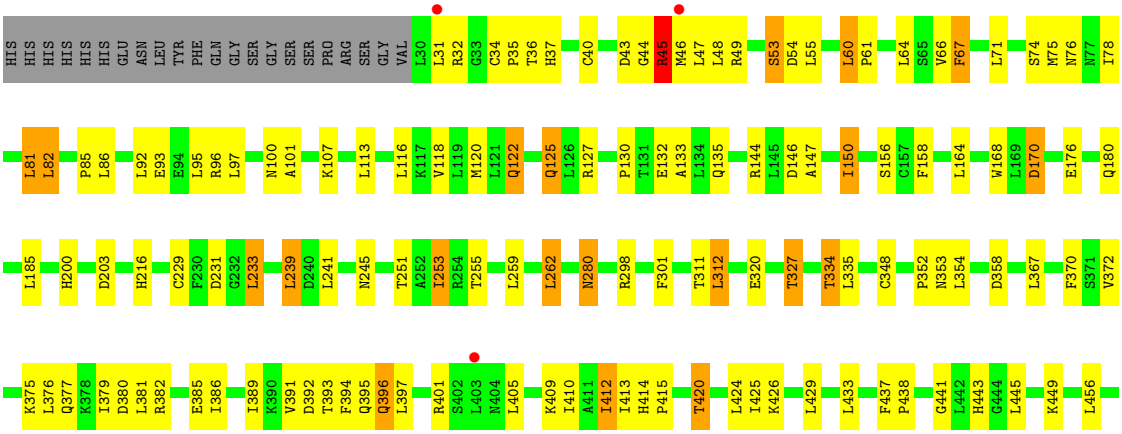
• Molecule 1: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR 5

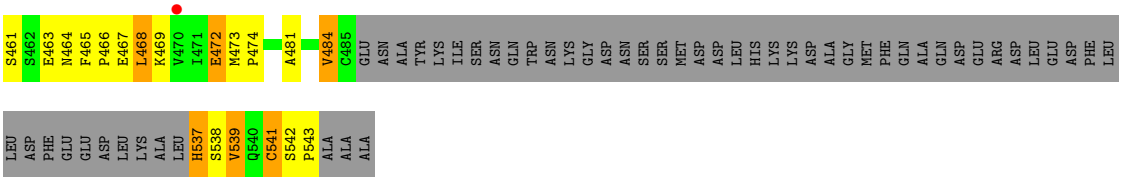
Chain E:



• Molecule 1: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR 5

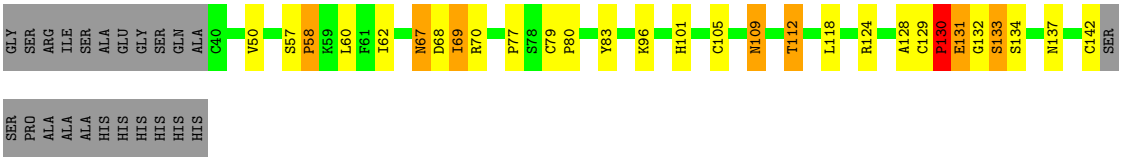
Chain F:





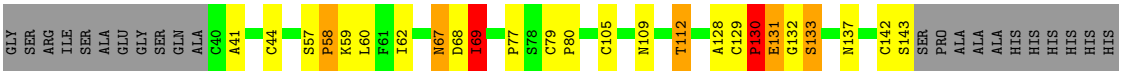
• Molecule 2: R-SPONDIN-1

Chain C:



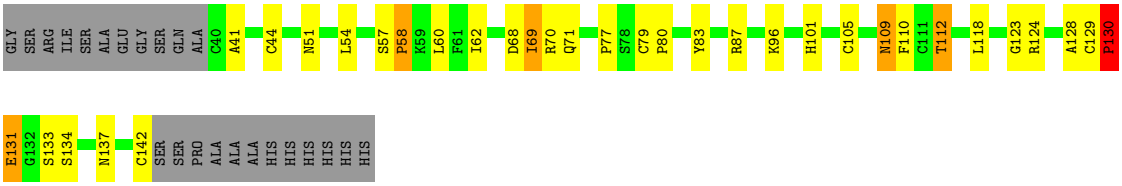
• Molecule 2: R-SPONDIN-1

Chain D:



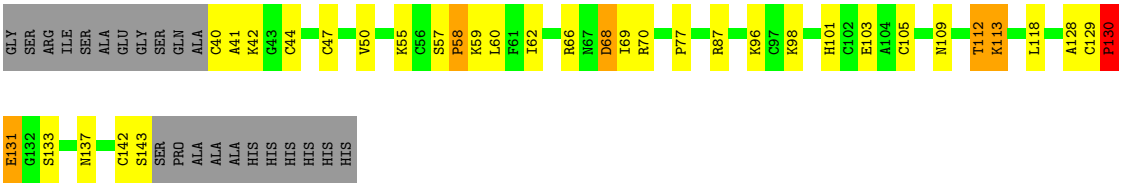
• Molecule 2: R-SPONDIN-1

Chain G:



• Molecule 2: R-SPONDIN-1

Chain H:

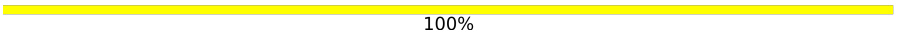


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

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

Chain J:



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

Chain K:

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

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	495.13Å 62.15Å 104.87Å 90.00° 91.19° 90.00°	Depositor
Resolution (Å)	65.50 – 3.20 65.50 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (65.50-3.20) 93.6 (65.50-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 3.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.240 , 0.287 0.233 , 0.280	Depositor DCC
R_{free} test set	2697 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	94.8	Xtriage
Anisotropy	0.938	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 104.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17955	wwPDB-VP
Average B, all atoms (Å^2)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.24	0/3808	0.54	3/5183 (0.1%)
1	B	0.24	0/3780	0.52	0/5146
1	E	0.24	0/3696	0.74	8/5033 (0.2%)
1	F	0.25	0/3710	0.53	0/5049
2	C	0.28	0/794	0.59	1/1066 (0.1%)
2	D	0.28	0/800	0.58	1/1074 (0.1%)
2	G	0.29	0/788	0.59	1/1059 (0.1%)
2	H	0.29	0/795	0.61	1/1067 (0.1%)
All	All	0.25	0/18171	0.59	15/24677 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	543	PRO	CA-C-O	-29.91	48.41	120.20
1	E	543	PRO	CA-C-N	15.20	150.63	117.20
1	E	543	PRO	O-C-N	-12.79	102.23	122.70
1	E	44	GLY	N-CA-C	-5.90	98.36	113.10
1	E	351	LEU	CA-CB-CG	5.70	128.41	115.30
1	A	81	LEU	CA-CB-CG	5.66	128.32	115.30
2	D	130	PRO	C-N-CA	5.60	135.69	121.70
1	E	81	LEU	CA-CB-CG	5.59	128.16	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	130	PRO	C-N-CA	5.56	135.60	121.70
2	H	130	PRO	C-N-CA	5.51	135.47	121.70
1	A	442	LEU	CA-CB-CG	5.47	127.88	115.30
2	C	130	PRO	C-N-CA	5.42	135.25	121.70
1	E	442	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	44	GLY	N-CA-C	-5.30	99.84	113.10
1	E	433	LEU	CA-CB-CG	5.23	127.33	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	543	PRO	Mainchain

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	3725	0	3727	71	0
1	B	3698	0	3704	85	0
1	E	3616	0	3613	87	0
1	F	3630	0	3635	86	0
2	C	778	0	744	16	0
2	D	784	0	749	12	0
2	G	772	0	733	20	0
2	H	779	0	738	20	0
3	I	28	0	25	0	0
4	J	39	0	34	0	0
4	K	39	0	34	0	0
4	L	39	0	34	1	0
5	B	14	0	13	0	0
5	F	14	0	13	0	0
All	All	17955	0	17796	379	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 11.

All (379) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ASP:OD2	1:E:270:ARG:NH2	2.12	0.83
1:A:231:ASP:HA	1:A:255:THR:HG21	1.60	0.83
1:F:484:VAL:HG21	1:F:541:CYS:HB3	1.61	0.81
2:C:50:VAL:HG23	2:C:70:ARG:HE	1.48	0.79
1:F:231:ASP:HA	1:F:255:THR:HG21	1.65	0.78
1:E:231:ASP:HA	1:E:255:THR:HG21	1.66	0.76
1:F:53:SER:O	1:F:55:LEU:N	2.23	0.70
1:F:43:ASP:HB2	1:F:49:ARG:HG3	1.72	0.70
1:F:82:LEU:HD13	1:F:85:PRO:HA	1.75	0.69
1:F:107:LYS:HG3	1:F:132:GLU:HB2	1.72	0.69
1:B:231:ASP:HA	1:B:255:THR:HG21	1.75	0.69
1:F:170:ASP:OD1	1:F:170:ASP:N	2.26	0.68
1:B:60:LEU:HG	1:B:82:LEU:HD21	1.76	0.68
1:B:170:ASP:N	1:B:170:ASP:OD1	2.27	0.67
1:F:469:LYS:HZ3	1:F:537:HIS:N	1.92	0.66
1:F:425:ILE:HG13	1:F:426:LYS:HG3	1.78	0.66
1:F:367:LEU:HD11	1:F:386:ILE:HD13	1.76	0.66
1:A:107:LYS:HG3	1:A:132:GLU:HB2	1.75	0.65
1:F:415:PRO:HA	1:F:438:PRO:HB3	1.79	0.65
1:E:107:LYS:HG3	1:E:132:GLU:HB2	1.77	0.65
1:A:82:LEU:HD13	1:A:85:PRO:HA	1.78	0.65
2:H:42:LYS:HD2	2:H:42:LYS:H	1.62	0.65
1:E:170:ASP:OD1	1:E:170:ASP:N	2.31	0.64
1:F:44:GLY:O	1:F:46:MET:N	2.30	0.64
2:C:109:ASN:OD1	2:C:124:ARG:NH2	2.30	0.64
1:B:53:SER:O	1:B:76:ASN:ND2	2.27	0.64
1:B:425:ILE:HG13	1:B:426:LYS:HG3	1.79	0.63
1:E:82:LEU:HD13	1:E:85:PRO:HA	1.80	0.63
1:F:60:LEU:HG	1:F:82:LEU:HD21	1.81	0.63
1:A:425:ILE:HG13	1:A:426:LYS:HG3	1.81	0.62
1:B:415:PRO:HA	1:B:438:PRO:HB3	1.82	0.62
1:E:486:GLU:N	1:E:486:GLU:OE1	2.32	0.62
2:C:130:PRO:HB3	2:C:131:GLU:HB2	1.80	0.62
1:F:395:GLN:OE1	1:F:420:THR:OG1	2.16	0.61
1:B:107:LYS:HG3	1:B:132:GLU:HB2	1.82	0.61
1:F:389:ILE:HD11	1:F:410:ILE:HD13	1.83	0.61
1:A:144:ARG:NH2	1:A:146:ASP:OD2	2.34	0.60
1:A:170:ASP:OD1	1:A:170:ASP:N	2.33	0.60
1:B:49:ARG:HG2	1:B:70:TYR:HB3	1.84	0.60
1:A:35:PRO:HG3	1:A:64:LEU:HD22	1.84	0.59
2:G:105:CYS:HA	2:G:112:THR:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:ARG:HG2	1:F:168:TRP:CE3	2.37	0.59
1:B:36:THR:O	1:B:37:HIS:HB2	2.02	0.59
1:E:367:LEU:HD11	1:E:386:ILE:HD13	1.83	0.58
1:E:144:ARG:HG2	1:E:168:TRP:CE3	2.38	0.58
2:G:130:PRO:HB3	2:G:131:GLU:HB2	1.85	0.58
1:A:144:ARG:HG2	1:A:168:TRP:CE3	2.39	0.57
1:B:45:ARG:O	1:B:46:MET:HB2	2.04	0.57
1:A:334:THR:HB	1:A:358:ASP:HB3	1.86	0.57
1:E:100:ASN:O	1:E:124:ASN:ND2	2.37	0.57
2:H:130:PRO:HB3	2:H:131:GLU:HB2	1.87	0.57
1:F:36:THR:O	1:F:37:HIS:HB2	2.05	0.57
1:E:392:ASP:HA	1:E:395:GLN:HG2	1.87	0.57
1:E:353:ASN:HA	1:E:375:LYS:HD3	1.87	0.56
2:G:83:TYR:CE1	2:G:96:LYS:HG2	2.40	0.56
1:A:164:LEU:HD23	1:A:185:LEU:HD22	1.86	0.56
1:A:327:THR:O	1:A:327:THR:OG1	2.24	0.56
1:B:367:LEU:HD11	1:B:386:ILE:HD13	1.86	0.56
1:E:36:THR:O	1:E:37:HIS:HB2	2.05	0.56
1:E:74:SER:O	1:E:76:ASN:ND2	2.39	0.56
1:F:74:SER:O	1:F:76:ASN:ND2	2.38	0.56
2:G:41:ALA:HB3	2:G:44:CYS:HB3	1.88	0.56
1:B:35:PRO:O	1:B:38:CYS:HB2	2.05	0.56
1:E:144:ARG:NH2	1:E:146:ASP:OD2	2.39	0.56
2:C:101:HIS:HB3	2:C:118:LEU:HD13	1.87	0.56
1:F:327:THR:O	1:F:327:THR:OG1	2.22	0.56
1:A:32:ARG:O	1:A:34:CYS:N	2.34	0.55
1:B:144:ARG:HG2	1:B:168:TRP:CE3	2.42	0.55
2:C:50:VAL:O	2:C:70:ARG:HD3	2.06	0.55
1:A:60:LEU:HG	1:A:82:LEU:HD21	1.88	0.55
2:C:60:LEU:HD22	2:C:77:PRO:HA	1.87	0.55
2:D:60:LEU:HD22	2:D:77:PRO:HA	1.88	0.55
1:E:463:GLU:O	1:E:464:ASN:HB2	2.07	0.55
1:E:296:VAL:HB	1:E:318:ILE:HD11	1.87	0.55
1:E:418:PHE:HA	1:E:421:LEU:HD13	1.89	0.55
1:B:348:CYS:SG	1:B:370:PHE:HA	2.47	0.55
1:B:253:ILE:O	1:B:280:ASN:ND2	2.33	0.54
1:E:66:VAL:O	1:E:67:PHE:HB2	2.08	0.54
1:E:391:VAL:HG22	1:E:414:HIS:CG	2.43	0.54
2:D:41:ALA:HB3	2:D:44:CYS:HB3	1.88	0.54
1:A:74:SER:O	1:A:76:ASN:ND2	2.41	0.54
1:A:100:ASN:O	1:A:124:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:LEU:HD21	1:E:262:LEU:HG	1.90	0.54
2:D:130:PRO:HB3	2:D:131:GLU:HB2	1.89	0.54
1:E:253:ILE:O	1:E:280:ASN:ND2	2.34	0.54
1:F:259:LEU:HD21	1:F:262:LEU:HG	1.88	0.53
1:A:36:THR:O	1:A:37:HIS:HB2	2.07	0.53
1:B:53:SER:O	1:B:55:LEU:N	2.39	0.53
1:B:334:THR:HB	1:B:358:ASP:HB3	1.90	0.53
1:E:479:CYS:HB3	1:E:484:VAL:HG23	1.89	0.53
1:B:144:ARG:NH2	1:B:146:ASP:OD2	2.41	0.53
1:B:377:GLN:OE1	1:B:401:ARG:NH2	2.41	0.53
2:H:60:LEU:HD22	2:H:77:PRO:HA	1.91	0.53
2:C:83:TYR:CE1	2:C:96:LYS:HG2	2.43	0.53
1:F:76:ASN:HB2	1:F:100:ASN:ND2	2.23	0.53
1:F:348:CYS:HB3	1:F:372:VAL:HB	1.90	0.53
1:A:60:LEU:HG	1:A:82:LEU:HD11	1.90	0.53
1:F:391:VAL:HG22	1:F:414:HIS:CG	2.43	0.53
1:B:43:ASP:HB2	1:B:49:ARG:HG3	1.90	0.53
1:B:389:ILE:HD11	1:B:410:ILE:HD13	1.91	0.53
1:F:101:ALA:HB1	1:F:125:GLN:HE22	1.72	0.53
1:F:53:SER:O	1:F:76:ASN:ND2	2.32	0.53
1:A:66:VAL:O	1:A:67:PHE:HB2	2.08	0.53
2:D:68:ASP:O	2:D:69:ILE:HG12	2.09	0.53
1:F:463:GLU:O	1:F:464:ASN:HB2	2.09	0.53
1:A:236:LEU:HD23	1:A:256:LEU:HD13	1.91	0.52
1:E:33:GLY:O	1:E:35:PRO:HD3	2.09	0.52
1:F:253:ILE:O	1:F:280:ASN:ND2	2.40	0.52
1:F:461:SER:HB3	2:G:54:LEU:HD11	1.90	0.52
1:A:367:LEU:HD11	1:A:386:ILE:HD13	1.90	0.52
1:A:463:GLU:O	1:A:464:ASN:HB2	2.08	0.52
1:A:471:ILE:O	1:A:541:CYS:HA	2.08	0.52
1:B:353:ASN:HA	1:B:375:LYS:HD3	1.90	0.52
1:F:164:LEU:HD23	1:F:185:LEU:HD22	1.91	0.52
1:B:158:PHE:HB3	1:B:185:LEU:HD21	1.92	0.52
1:E:233:LEU:HD13	1:E:233:LEU:H	1.75	0.52
2:C:105:CYS:HA	2:C:112:THR:H	1.74	0.52
1:E:164:LEU:HD23	1:E:185:LEU:HD22	1.91	0.52
1:F:146:ASP:OD2	2:H:87:ARG:NH1	2.43	0.52
1:F:441:GLY:O	1:F:443:HIS:N	2.43	0.52
2:H:41:ALA:HB3	2:H:44:CYS:HB3	1.92	0.52
1:F:538:SER:O	1:F:539:VAL:HG22	2.10	0.52
1:E:485:CYS:O	2:H:66:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:392:ASP:HA	1:F:395:GLN:HG2	1.92	0.51
1:B:74:SER:O	1:B:76:ASN:ND2	2.42	0.51
1:B:317:GLN:HG3	1:F:200:HIS:CE1	2.46	0.51
1:F:78:ILE:HB	1:F:100:ASN:HB3	1.91	0.51
1:A:400:LEU:HD23	1:A:421:LEU:HD23	1.92	0.51
1:B:236:LEU:HD23	1:B:256:LEU:HD13	1.92	0.51
1:E:81:LEU:HB2	1:E:82:LEU:HD12	1.93	0.51
1:E:376:LEU:HD23	1:E:379:ILE:HD11	1.92	0.51
1:B:144:ARG:HA	1:B:168:TRP:HB2	1.93	0.51
1:F:53:SER:C	1:F:76:ASN:HD21	2.13	0.51
1:B:66:VAL:O	1:B:67:PHE:HB2	2.11	0.51
1:B:463:GLU:O	1:B:464:ASN:HB2	2.10	0.51
1:A:393:THR:HG23	1:A:394:PHE:CD2	2.46	0.51
1:B:101:ALA:HB1	1:B:125:GLN:HE22	1.75	0.51
1:E:90:ARG:HD2	1:E:90:ARG:N	2.26	0.51
1:E:158:PHE:HB3	1:E:185:LEU:HD21	1.93	0.51
2:G:60:LEU:HD22	2:G:77:PRO:HA	1.94	0.50
1:B:76:ASN:HB2	1:B:100:ASN:ND2	2.27	0.50
1:A:130:PRO:HB3	1:A:133:ALA:HB3	1.93	0.50
1:F:130:PRO:HB3	1:F:133:ALA:HB3	1.92	0.50
1:F:465:PHE:CD1	1:F:468:LEU:HD21	2.47	0.50
1:A:144:ARG:HA	1:A:168:TRP:HB2	1.94	0.50
1:E:425:ILE:HG13	1:E:426:LYS:HG3	1.94	0.50
1:A:237:GLU:OE1	2:C:124:ARG:NH1	2.45	0.50
1:E:327:THR:O	1:E:327:THR:OG1	2.25	0.50
2:H:101:HIS:HB3	2:H:118:LEU:HD13	1.93	0.50
1:F:31:LEU:O	1:F:32:ARG:HB2	2.12	0.49
1:E:348:CYS:HB3	1:E:372:VAL:HB	1.93	0.49
1:B:327:THR:O	1:B:327:THR:OG1	2.23	0.49
1:B:82:LEU:HD13	1:B:85:PRO:HA	1.94	0.49
1:A:466:PRO:O	1:A:467:GLU:HB2	2.13	0.49
1:E:144:ARG:HA	1:E:168:TRP:HB2	1.95	0.49
2:C:67:ASN:OD1	2:C:67:ASN:N	2.44	0.49
1:A:238:THR:HG22	1:A:261:GLU:HB3	1.94	0.49
1:B:117:LYS:HE3	1:B:141:GLN:HE21	1.78	0.49
1:A:312:LEU:HB3	1:A:335:LEU:HD13	1.94	0.49
1:B:294:GLN:HB3	1:B:317:GLN:HG2	1.94	0.49
1:B:393:THR:HG23	1:B:394:PHE:CD2	2.48	0.49
1:E:541:CYS:CB	1:E:542:SER:HA	2.43	0.49
1:E:541:CYS:HB3	1:E:542:SER:HA	1.95	0.49
1:A:284:ILE:HG22	1:A:285:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:ARG:HA	1:B:120:MET:HB2	1.94	0.48
1:E:60:LEU:HG	1:E:82:LEU:HD21	1.95	0.48
1:E:541:CYS:HB3	1:E:542:SER:CA	2.43	0.48
1:F:146:ASP:OD1	1:F:146:ASP:N	2.45	0.48
1:E:236:LEU:HD23	1:E:256:LEU:HD13	1.94	0.48
2:H:40:CYS:SG	2:H:47:CYS:N	2.86	0.48
1:E:294:GLN:HB3	1:E:317:GLN:HG2	1.95	0.48
1:E:334:THR:HB	1:E:358:ASP:HB3	1.95	0.48
1:F:203:ASP:HA	1:F:229:CYS:HA	1.94	0.48
1:A:158:PHE:HB3	1:A:185:LEU:HD21	1.96	0.48
1:B:391:VAL:HG22	1:B:414:HIS:CG	2.49	0.48
1:B:441:GLY:O	1:B:443:HIS:N	2.46	0.48
1:F:66:VAL:O	1:F:67:PHE:HB2	2.14	0.48
2:G:70:ARG:NH1	2:G:70:ARG:HB3	2.28	0.48
1:A:391:VAL:HG22	1:A:414:HIS:CG	2.49	0.48
1:A:81:LEU:HB2	1:A:82:LEU:HD12	1.94	0.48
1:A:200:HIS:CE1	1:E:317:GLN:HG3	2.48	0.48
1:B:233:LEU:HD13	1:B:233:LEU:H	1.78	0.48
1:B:465:PHE:CD1	1:B:468:LEU:HD21	2.49	0.48
1:E:90:ARG:HD2	1:E:90:ARG:H	1.79	0.48
1:E:312:LEU:HB3	1:E:335:LEU:HD13	1.95	0.48
1:F:44:GLY:O	1:F:47:LEU:N	2.44	0.48
1:E:270:ARG:NH1	1:E:292:PRO:HB2	2.29	0.47
1:E:348:CYS:SG	1:E:370:PHE:HA	2.54	0.47
1:F:158:PHE:HB3	1:F:185:LEU:HD21	1.95	0.47
1:B:389:ILE:HD12	1:B:413:ILE:HG12	1.96	0.47
1:A:391:VAL:HG22	1:A:414:HIS:CD2	2.50	0.47
1:F:481:ALA:O	2:G:51:ASN:ND2	2.36	0.47
1:E:393:THR:HG23	1:E:394:PHE:CD2	2.49	0.47
1:F:376:LEU:HD23	1:F:379:ILE:HD11	1.94	0.47
1:A:31:LEU:O	1:A:32:ARG:HB2	2.14	0.47
1:B:35:PRO:HB3	1:B:61:PRO:HG2	1.97	0.47
1:E:146:ASP:OD1	1:E:146:ASP:N	2.46	0.47
1:F:465:PHE:HB3	1:F:468:LEU:HG	1.97	0.47
2:G:134:SER:HB3	2:G:142:CYS:HB3	1.95	0.47
2:D:105:CYS:HA	2:D:112:THR:H	1.79	0.47
1:F:393:THR:HG23	1:F:394:PHE:CD2	2.49	0.47
1:F:396:GLN:HE22	1:F:420:THR:HG21	1.80	0.47
2:H:70:ARG:HH11	2:H:70:ARG:HG2	1.79	0.47
1:A:130:PRO:HB2	1:A:134:LEU:HG	1.95	0.47
1:B:348:CYS:HB3	1:B:372:VAL:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:233:LEU:HD13	1:F:233:LEU:H	1.80	0.47
1:A:418:PHE:HA	1:A:421:LEU:HD13	1.96	0.47
1:F:81:LEU:HA	1:F:82:LEU:HG	1.97	0.47
1:F:147:ALA:HB1	2:H:59:LYS:HG2	1.96	0.47
1:F:445:LEU:O	1:F:468:LEU:HD22	2.15	0.46
1:F:334:THR:HB	1:F:358:ASP:HB3	1.97	0.46
1:F:353:ASN:HA	1:F:375:LYS:HD3	1.96	0.46
2:G:101:HIS:HB3	2:G:118:LEU:HD13	1.97	0.46
1:E:194:ALA:O	1:E:196:ASN:ND2	2.48	0.46
1:F:96:ARG:HA	1:F:120:MET:HB2	1.97	0.46
1:F:135:GLN:NE2	1:F:156:SER:O	2.48	0.46
1:A:148:ASN:HB2	1:A:150:ILE:HG23	1.98	0.46
1:B:425:ILE:O	1:B:446:THR:N	2.49	0.46
1:B:376:LEU:HD23	1:B:379:ILE:HD11	1.97	0.46
1:E:238:THR:HG21	2:G:109:ASN:ND2	2.30	0.46
1:B:370:PHE:O	1:B:397:LEU:HD21	2.16	0.46
1:A:348:CYS:SG	1:A:370:PHE:HA	2.55	0.46
1:B:78:ILE:HB	1:B:100:ASN:HB3	1.97	0.46
2:C:68:ASP:C	2:C:70:ARG:H	2.18	0.46
1:E:400:LEU:HD23	1:E:421:LEU:HD23	1.97	0.46
1:F:144:ARG:HA	1:F:168:TRP:HB2	1.97	0.46
1:B:392:ASP:HA	1:B:395:GLN:HG2	1.97	0.46
1:E:201:ILE:HG22	1:E:229:CYS:HB2	1.98	0.46
1:E:441:GLY:O	1:E:443:HIS:N	2.48	0.46
1:E:487:ASN:N	1:E:487:ASN:OD1	2.49	0.46
1:F:449:LYS:HG2	1:F:472:GLU:HG3	1.96	0.46
2:D:67:ASN:N	2:D:67:ASN:OD1	2.48	0.45
2:D:143:SER:O	2:D:143:SER:OG	2.33	0.45
1:A:376:LEU:HD23	1:A:379:ILE:HD11	1.96	0.45
1:B:43:ASP:OD1	1:B:44:GLY:N	2.49	0.45
1:E:50:VAL:HB	1:E:71:LEU:HD23	1.98	0.45
1:E:60:LEU:HG	1:E:82:LEU:HD11	1.98	0.45
1:E:146:ASP:OD2	2:G:87:ARG:NH1	2.48	0.45
1:E:148:ASN:HB2	1:E:150:ILE:HG23	1.99	0.45
1:A:441:GLY:O	1:A:443:HIS:N	2.50	0.45
1:F:466:PRO:O	1:F:467:GLU:HB2	2.17	0.45
1:A:194:ALA:O	1:A:196:ASN:ND2	2.49	0.45
1:B:164:LEU:HD23	1:B:185:LEU:HD22	1.98	0.45
1:B:239:LEU:HD22	1:B:241:LEU:HG	1.98	0.45
1:E:415:PRO:HA	1:E:438:PRO:HB3	1.97	0.45
1:B:180:GLN:H	1:B:180:GLN:HG3	1.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLN:HE21	1:A:144:ARG:HD3	1.81	0.45
1:B:351:LEU:HD13	1:B:354:LEU:HD22	1.98	0.45
1:F:144:ARG:NH2	1:F:146:ASP:OD2	2.50	0.45
1:A:203:ASP:HA	1:A:229:CYS:HA	1.98	0.45
1:B:43:ASP:HA	1:B:49:ARG:HD3	1.99	0.45
1:B:259:LEU:HD21	1:B:262:LEU:HG	1.98	0.44
1:E:238:THR:HG21	2:G:109:ASN:HD21	1.81	0.44
1:E:270:ARG:HH11	1:E:292:PRO:HB2	1.82	0.44
1:A:348:CYS:HB3	1:A:372:VAL:HB	1.98	0.44
1:E:466:PRO:O	1:E:467:GLU:HB2	2.17	0.44
1:E:127:ARG:C	1:E:150:ILE:HA	2.37	0.44
1:F:385:GLU:OE1	1:F:409:LYS:NZ	2.49	0.44
1:A:408:ASN:HB2	1:A:432:ASN:OD1	2.17	0.44
1:B:47:LEU:HD13	1:B:69:SER:HB3	2.00	0.44
2:H:143:SER:O	2:H:143:SER:OG	2.35	0.44
1:F:312:LEU:HB3	1:F:335:LEU:HD13	2.00	0.44
2:H:50:VAL:HG23	2:H:70:ARG:HD3	1.99	0.44
2:H:103:GLU:OE1	2:H:113:LYS:NZ	2.47	0.44
1:E:130:PRO:HB2	1:E:134:LEU:HG	1.98	0.44
1:F:301:PHE:O	1:F:327:THR:HG21	2.18	0.44
2:G:68:ASP:O	2:G:69:ILE:HG22	2.16	0.44
1:B:284:ILE:HG22	1:B:285:THR:HG23	2.00	0.44
1:F:381:LEU:HB2	1:F:405:LEU:HD23	2.00	0.44
2:G:109:ASN:OD1	2:G:124:ARG:NH2	2.50	0.44
2:D:79:CYS:HA	2:D:80:PRO:HD3	1.88	0.44
2:H:70:ARG:HG2	2:H:70:ARG:NH1	2.33	0.44
1:A:90:ARG:HD3	1:A:91:PHE:CE2	2.53	0.43
1:A:238:THR:HG21	2:C:109:ASN:ND2	2.32	0.43
1:E:130:PRO:HB3	1:E:133:ALA:HB3	2.00	0.43
2:G:79:CYS:HA	2:G:80:PRO:HD3	1.89	0.43
1:A:437:PHE:HA	1:A:438:PRO:HD3	1.83	0.43
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.87	0.43
1:A:392:ASP:HA	1:A:395:GLN:HG2	1.99	0.43
2:H:68:ASP:HA	2:H:69:ILE:HA	1.70	0.43
1:A:122:GLN:NE2	1:A:144:ARG:HD3	2.33	0.43
1:A:81:LEU:HD11	1:A:105:ILE:HD13	2.00	0.43
1:E:43:ASP:HB2	1:E:49:ARG:HG3	1.99	0.43
2:H:50:VAL:HG21	2:H:70:ARG:NH1	2.33	0.43
1:B:57:LEU:HB3	1:B:59:GLU:O	2.17	0.43
1:B:395:GLN:OE1	1:B:420:THR:OG1	2.25	0.43
1:E:284:ILE:HG22	1:E:285:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:MET:C	1:F:76:ASN:HD22	2.21	0.43
1:F:370:PHE:O	1:F:397:LEU:HD21	2.19	0.43
1:B:468:LEU:HD12	1:B:471:ILE:HG12	2.01	0.43
1:F:437:PHE:HA	1:F:438:PRO:HD3	1.86	0.43
1:A:50:VAL:HB	1:A:71:LEU:HD23	2.01	0.43
1:E:75:MET:C	1:E:76:ASN:HD22	2.22	0.43
1:A:439:ILE:HD12	1:A:442:LEU:HD11	2.01	0.43
1:A:75:MET:C	1:A:76:ASN:HD22	2.21	0.42
1:B:75:MET:C	1:B:76:ASN:HD22	2.22	0.42
1:B:147:ALA:HB1	2:D:59:LYS:HG2	2.01	0.42
2:C:134:SER:HB3	2:C:142:CYS:HB3	2.00	0.42
1:E:324:LEU:HD13	1:E:330:LEU:HD12	2.00	0.42
1:F:352:PRO:C	1:F:354:LEU:H	2.23	0.42
1:B:437:PHE:HA	1:B:438:PRO:HD3	1.89	0.42
1:E:122:GLN:NE2	1:E:144:ARG:HD3	2.33	0.42
1:B:107:LYS:CG	1:B:132:GLU:HB2	2.50	0.42
1:E:96:ARG:HA	1:E:120:MET:HB2	2.00	0.42
1:F:127:ARG:C	1:F:150:ILE:HA	2.39	0.42
1:B:47:LEU:HD23	1:B:47:LEU:HA	1.74	0.42
1:B:203:ASP:HA	1:B:229:CYS:HA	2.01	0.42
1:B:466:PRO:O	1:B:467:GLU:HB2	2.19	0.42
2:C:79:CYS:HA	2:C:80:PRO:HD3	1.84	0.42
1:E:304:LEU:H	1:E:327:THR:HB	1.84	0.42
1:A:57:LEU:HB3	1:A:59:GLU:O	2.20	0.42
1:B:324:LEU:HD13	1:B:330:LEU:HD12	2.02	0.42
1:F:47:LEU:HA	1:F:47:LEU:HD23	1.72	0.42
1:F:377:GLN:OE1	1:F:401:ARG:NH2	2.53	0.42
1:A:272:ILE:HB	1:A:296:VAL:HG22	2.01	0.42
1:B:171:ASP:OD2	2:D:59:LYS:HE3	2.19	0.42
1:B:373:CYS:O	1:B:376:LEU:HB2	2.20	0.42
1:E:312:LEU:HD13	1:E:312:LEU:HA	1.90	0.42
1:A:97:LEU:HD12	1:A:97:LEU:HA	1.82	0.42
1:B:344:PRO:O	1:B:347:VAL:HG23	2.19	0.42
1:F:298:ARG:HD3	1:F:320:GLU:HB2	2.02	0.42
1:A:233:LEU:HD13	1:A:233:LEU:H	1.85	0.42
1:B:66:VAL:HA	1:B:89:LEU:HD22	2.02	0.42
1:B:194:ALA:O	1:B:196:ASN:ND2	2.53	0.42
2:D:57:SER:HB2	2:D:58:PRO:HD2	2.00	0.42
1:E:381:LEU:HB2	1:E:405:LEU:HD23	2.01	0.42
2:H:57:SER:HB2	2:H:58:PRO:HD2	2.00	0.42
1:A:323:ASP:OD1	1:A:325:THR:OG1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:132:GLY:O	2:D:133:SER:HB3	2.19	0.41
1:E:471:ILE:O	1:E:541:CYS:HA	2.20	0.41
1:F:412:ILE:HG12	1:F:413:ILE:N	2.34	0.41
1:F:441:GLY:C	1:F:443:HIS:H	2.24	0.41
1:B:72:ASP:HA	1:B:96:ARG:HB2	2.02	0.41
1:B:127:ARG:C	1:B:150:ILE:HA	2.40	0.41
1:E:78:ILE:O	1:E:102:LEU:HD23	2.20	0.41
1:F:122:GLN:NE2	1:F:144:ARG:HD3	2.35	0.41
1:F:239:LEU:HD22	1:F:241:LEU:HG	2.02	0.41
1:F:542:SER:HA	1:F:543:PRO:HD3	1.94	0.41
2:H:105:CYS:HA	2:H:112:THR:H	1.85	0.41
1:B:122:GLN:NE2	1:B:144:ARG:HD3	2.36	0.41
1:B:249:PHE:CZ	1:B:276:ALA:HB1	2.55	0.41
1:B:405:LEU:HB2	1:B:429:LEU:HD23	2.02	0.41
1:B:479:CYS:HB2	1:B:484:VAL:O	2.20	0.41
2:C:57:SER:HB2	2:C:58:PRO:HD2	2.01	0.41
1:E:147:ALA:HB2	2:G:87:ARG:CZ	2.51	0.41
1:E:408:ASN:HB2	1:E:432:ASN:OD1	2.20	0.41
1:A:275:LYS:HE3	1:F:298:ARG:HH12	1.85	0.41
1:E:64:LEU:HB3	1:E:86:LEU:HD22	2.02	0.41
1:E:188:LEU:HD23	1:E:188:LEU:HA	1.95	0.41
1:A:259:LEU:HD21	1:A:262:LEU:HG	2.01	0.41
1:A:405:LEU:HB2	1:A:429:LEU:HD23	2.03	0.41
1:E:296:VAL:HG21	1:E:312:LEU:HD11	2.02	0.41
1:E:370:PHE:O	1:E:397:LEU:HD21	2.19	0.41
1:E:421:LEU:HD22	1:E:424:LEU:HD12	2.03	0.41
2:H:96:LYS:HE2	2:H:98:LYS:HE3	2.03	0.41
1:A:182:PHE:HA	1:A:185:LEU:HD12	2.03	0.41
1:B:296:VAL:HB	1:B:318:ILE:HD11	2.02	0.41
1:B:323:ASP:OD1	1:B:325:THR:OG1	2.36	0.41
1:F:473:MET:HG3	1:F:474:PRO:HD2	2.02	0.41
1:A:74:SER:HA	1:A:98:ALA:O	2.21	0.41
1:E:373:CYS:O	1:E:376:LEU:HB2	2.21	0.41
1:B:34:CYS:O	1:B:36:THR:N	2.54	0.40
1:B:352:PRO:C	1:B:354:LEU:H	2.24	0.40
1:E:122:GLN:HE21	1:E:144:ARG:HD3	1.86	0.40
1:E:301:PHE:O	1:E:327:THR:HG21	2.22	0.40
2:G:57:SER:HB2	2:G:58:PRO:HD2	2.03	0.40
4:L:1:NAG:H4	4:L:2:NAG:H2	1.78	0.40
1:A:218:HIS:ND1	1:A:240:ASP:OD2	2.52	0.40
1:E:486:GLU:O	2:H:66:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:LEU:HD11	1:F:82:LEU:HD11	2.03	0.40
2:G:110:PHE:CD2	2:G:123:GLY:HA3	2.57	0.40
1:F:44:GLY:O	1:F:45:ARG:C	2.59	0.40
1:A:433:LEU:HD22	1:B:290:ASP:CG	2.41	0.40
2:C:132:GLY:O	2:C:133:SER:HB3	2.22	0.40
1:F:34:CYS:SG	1:F:40:CYS:N	2.94	0.40
1:F:348:CYS:SG	1:F:370:PHE:HA	2.61	0.40
1:F:380:ASP:OD1	1:F:382:ARG:HG2	2.22	0.40
1:F:405:LEU:HB2	1:F:429:LEU:HD23	2.04	0.40
2:G:130:PRO:CB	2:G:131:GLU:HB2	2.51	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	470/539 (87%)	424 (90%)	44 (9%)	2 (0%)	30 64
1	B	467/539 (87%)	406 (87%)	52 (11%)	9 (2%)	6 34
1	E	458/539 (85%)	415 (91%)	39 (8%)	4 (1%)	14 49
1	F	459/539 (85%)	407 (89%)	43 (9%)	9 (2%)	6 32
2	C	101/126 (80%)	86 (85%)	7 (7%)	8 (8%)	1 5
2	D	102/126 (81%)	86 (84%)	7 (7%)	9 (9%)	0 3
2	G	101/126 (80%)	85 (84%)	8 (8%)	8 (8%)	1 5
2	H	102/126 (81%)	84 (82%)	9 (9%)	9 (9%)	0 3
All	All	2260/2660 (85%)	1993 (88%)	209 (9%)	58 (3%)	4 27

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	35	PRO
1	B	36	THR
2	C	69	ILE
2	C	128	ALA
2	C	129	CYS
2	C	130	PRO
2	C	133	SER
2	D	128	ALA
2	D	129	CYS
2	D	130	PRO
2	D	133	SER
1	F	45	ARG
1	F	54	ASP
1	F	539	VAL
2	G	128	ALA
2	G	129	CYS
2	G	130	PRO
2	G	133	SER
2	H	128	ALA
2	H	129	CYS
2	H	130	PRO
2	H	133	SER
1	B	53	SER
1	B	530	GLU
1	B	541	CYS
2	C	131	GLU
2	C	137	ASN
2	D	69	ILE
2	D	131	GLU
2	D	137	ASN
1	E	484	VAL
1	E	486	GLU
1	F	53	SER
2	G	69	ILE
2	G	131	GLU
2	H	68	ASP
2	H	131	GLU
2	H	137	ASN
1	B	54	ASP
1	B	67	PHE
2	D	142	CYS
1	E	485	CYS
1	F	35	PRO

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Mol	Chain	Res	Type
2	G	137	ASN
2	H	142	CYS
1	A	35	PRO
1	B	61	PRO
1	F	67	PHE
1	A	33	GLY
1	F	61	PRO
1	F	541	CYS
1	B	253	ILE
1	F	253	ILE
2	C	58	PRO
1	E	253	ILE
2	H	58	PRO
2	D	58	PRO
2	G	58	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	429/484 (89%)	392 (91%)	37 (9%)	8 33
1	B	427/484 (88%)	388 (91%)	39 (9%)	7 29
1	E	416/484 (86%)	383 (92%)	33 (8%)	10 38
1	F	418/484 (86%)	376 (90%)	42 (10%)	6 26
2	C	89/105 (85%)	84 (94%)	5 (6%)	17 50
2	D	90/105 (86%)	85 (94%)	5 (6%)	17 50
2	G	88/105 (84%)	84 (96%)	4 (4%)	23 56
2	H	88/105 (84%)	83 (94%)	5 (6%)	17 50
All	All	2045/2356 (87%)	1875 (92%)	170 (8%)	9 35

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	46	MET
1	A	48	LEU
1	A	54	ASP
1	A	60	LEU
1	A	64	LEU
1	A	71	LEU
1	A	81	LEU
1	A	82	LEU
1	A	90	ARG
1	A	92	LEU
1	A	93	GLU
1	A	95	LEU
1	A	97	LEU
1	A	113	LEU
1	A	116	LEU
1	A	118	VAL
1	A	122	GLN
1	A	138	ARG
1	A	150	ILE
1	A	170	ASP
1	A	216	HIS
1	A	227	LYS
1	A	233	LEU
1	A	239	LEU
1	A	262	LEU
1	A	280	ASN
1	A	312	LEU
1	A	327	THR
1	A	334	THR
1	A	351	LEU
1	A	356	VAL
1	A	423	SER
1	A	424	LEU
1	A	433	LEU
1	A	456	LEU
1	A	472	GLU
1	B	36	THR
1	B	48	LEU
1	B	60	LEU
1	B	64	LEU
1	B	71	LEU
1	B	81	LEU

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Mol	Chain	Res	Type
1	B	82	LEU
1	B	92	LEU
1	B	93	GLU
1	B	95	LEU
1	B	113	LEU
1	B	116	LEU
1	B	118	VAL
1	B	122	GLN
1	B	125	GLN
1	B	150	ILE
1	B	165	ARG
1	B	170	ASP
1	B	180	GLN
1	B	216	HIS
1	B	227	LYS
1	B	233	LEU
1	B	239	LEU
1	B	251	THR
1	B	262	LEU
1	B	280	ASN
1	B	312	LEU
1	B	327	THR
1	B	334	THR
1	B	396	GLN
1	B	420	THR
1	B	424	LEU
1	B	433	LEU
1	B	456	LEU
1	B	468	LEU
1	B	472	GLU
1	B	479	CYS
1	B	480	CYS
1	B	528	ASP
2	C	62	ILE
2	C	67	ASN
2	C	69	ILE
2	C	109	ASN
2	C	112	THR
2	D	62	ILE
2	D	67	ASN
2	D	69	ILE
2	D	109	ASN

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Mol	Chain	Res	Type
2	D	112	THR
1	E	48	LEU
1	E	54	ASP
1	E	60	LEU
1	E	64	LEU
1	E	71	LEU
1	E	81	LEU
1	E	82	LEU
1	E	90	ARG
1	E	92	LEU
1	E	93	GLU
1	E	95	LEU
1	E	113	LEU
1	E	116	LEU
1	E	118	VAL
1	E	122	GLN
1	E	138	ARG
1	E	150	ILE
1	E	170	ASP
1	E	227	LYS
1	E	233	LEU
1	E	239	LEU
1	E	262	LEU
1	E	280	ASN
1	E	312	LEU
1	E	327	THR
1	E	334	THR
1	E	351	LEU
1	E	424	LEU
1	E	433	LEU
1	E	456	LEU
1	E	472	GLU
1	E	541	CYS
1	E	542	SER
1	F	45	ARG
1	F	48	LEU
1	F	60	LEU
1	F	64	LEU
1	F	71	LEU
1	F	81	LEU
1	F	82	LEU
1	F	86	LEU

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Mol	Chain	Res	Type
1	F	92	LEU
1	F	93	GLU
1	F	95	LEU
1	F	97	LEU
1	F	113	LEU
1	F	116	LEU
1	F	118	VAL
1	F	122	GLN
1	F	125	GLN
1	F	150	ILE
1	F	170	ASP
1	F	176	GLU
1	F	180	GLN
1	F	216	HIS
1	F	233	LEU
1	F	239	LEU
1	F	245	ASN
1	F	251	THR
1	F	262	LEU
1	F	280	ASN
1	F	311	THR
1	F	312	LEU
1	F	327	THR
1	F	334	THR
1	F	396	GLN
1	F	412	ILE
1	F	420	THR
1	F	424	LEU
1	F	433	LEU
1	F	456	LEU
1	F	468	LEU
1	F	472	GLU
1	F	484	VAL
1	F	537	HIS
2	G	62	ILE
2	G	71	GLN
2	G	109	ASN
2	G	112	THR
2	H	55	LYS
2	H	62	ILE
2	H	109	ASN
2	H	112	THR

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Mol	Chain	Res	Type
2	H	113	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	302	GLN
1	B	100	ASN
1	B	141	GLN
1	E	76	ASN
1	E	216	HIS
1	F	76	ASN
1	F	100	ASN
1	F	122	GLN
1	F	125	GLN
1	F	355	GLN

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

11 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	0.29	0	17,19,21	0.85	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	I	2	3	14,14,15	0.42	0	17,19,21	0.58	0
4	NAG	J	1	4,1	14,14,15	1.13	2 (14%)	17,19,21	0.77	0
4	NAG	J	2	4	14,14,15	1.06	1 (7%)	17,19,21	0.86	0
4	BMA	J	3	4	11,11,12	0.66	0	15,15,17	1.38	3 (20%)
4	NAG	K	1	4,1	14,14,15	0.66	1 (7%)	17,19,21	0.48	0
4	NAG	K	2	4	14,14,15	0.28	0	17,19,21	0.55	0
4	BMA	K	3	4	11,11,12	0.95	0	15,15,17	0.92	0
4	NAG	L	1	4,1	14,14,15	0.58	0	17,19,21	1.13	1 (5%)
4	NAG	L	2	4	14,14,15	0.73	1 (7%)	17,19,21	0.90	1 (5%)
4	BMA	L	3	4	11,11,12	0.93	1 (9%)	15,15,17	1.39	1 (6%)

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	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	NAG	K	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
4	NAG	L	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	3/6/23/26	0/1/1/1
4	BMA	L	3	4	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	2	NAG	O5-C1	-3.82	1.37	1.43
4	J	1	NAG	O5-C1	3.42	1.49	1.43
4	J	1	NAG	C1-C2	2.36	1.55	1.52
4	L	2	NAG	C1-C2	2.30	1.55	1.52
4	L	3	BMA	O5-C5	2.19	1.47	1.43
4	K	1	NAG	C1-C2	2.15	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	3	BMA	C1-O5-C5	4.63	118.46	112.19
4	L	1	NAG	C1-O5-C5	3.98	117.58	112.19
4	J	3	BMA	C1-O5-C5	3.45	116.87	112.19
4	J	3	BMA	O5-C1-C2	2.63	114.82	110.77
4	L	2	NAG	C1-O5-C5	2.41	115.45	112.19
4	J	3	BMA	C1-C2-C3	2.25	112.43	109.67
3	I	1	NAG	O4-C4-C5	2.07	114.44	109.30
3	I	1	NAG	C1-O5-C5	2.06	114.98	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	3	BMA	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	K	3	BMA	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
4	L	2	NAG	C1-C2-N2-C7

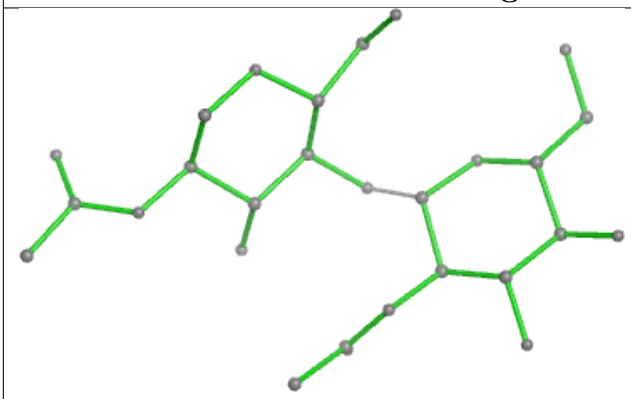
There are no ring outliers.

2 monomers are involved in 1 short contact:

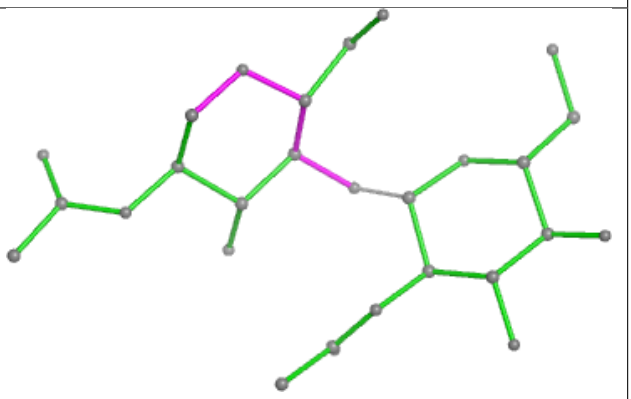
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1	NAG	1	0
4	L	2	NAG	1	0

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

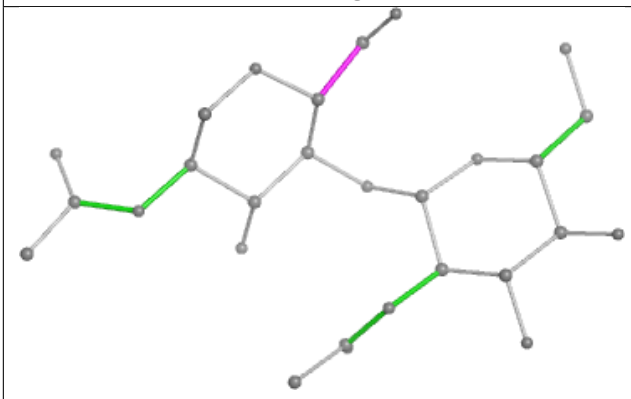
Oligosaccharide Chain I



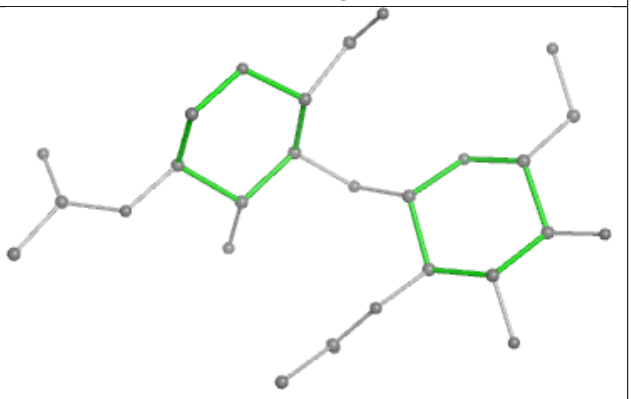
Bond lengths



Bond angles

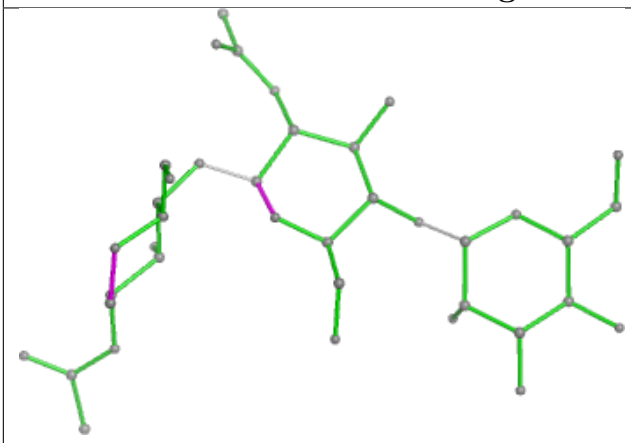


Torsions

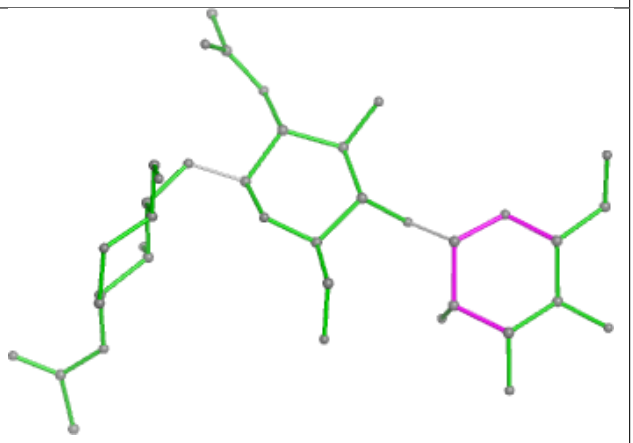


Rings

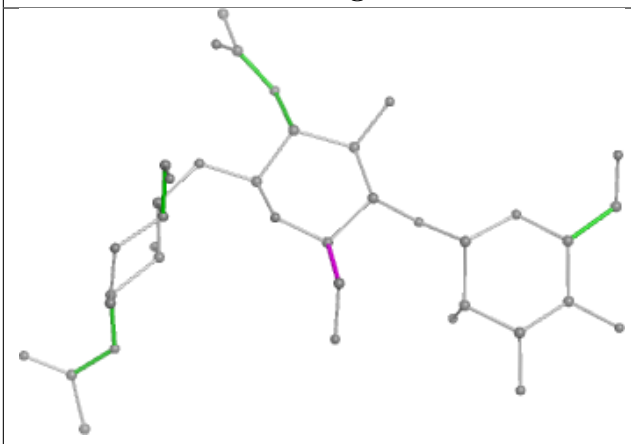
Oligosaccharide Chain J



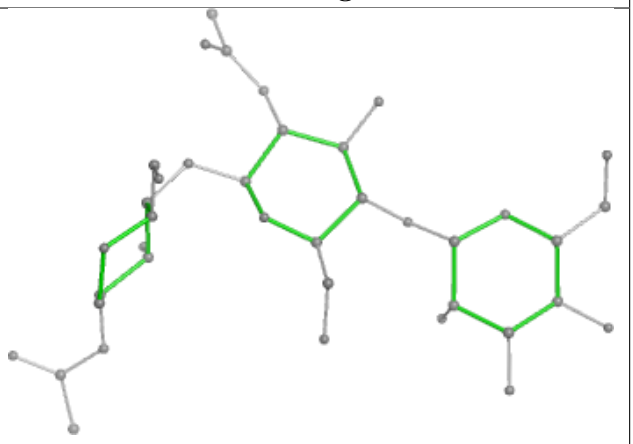
Bond lengths



Bond angles

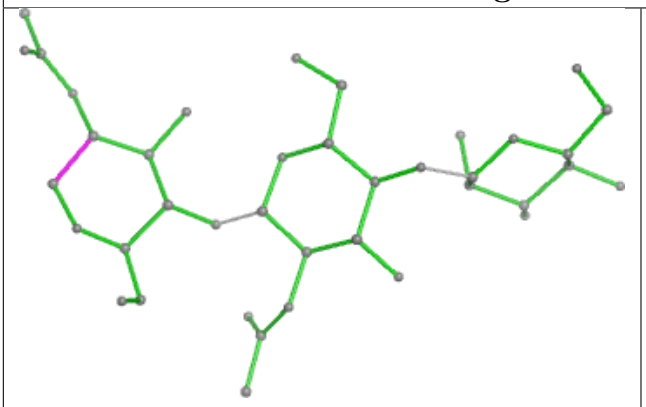


Torsions

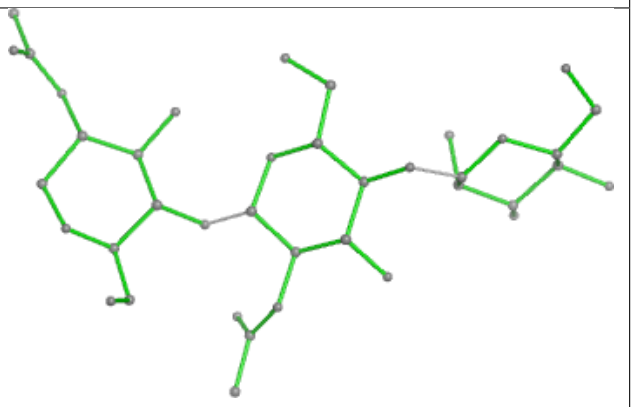


Rings

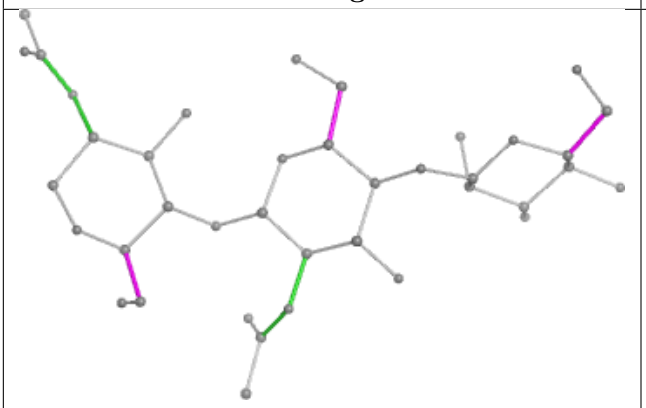
Oligosaccharide Chain K



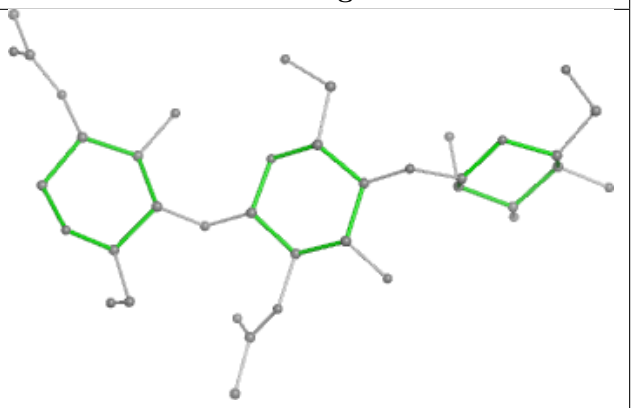
Bond lengths



Bond angles

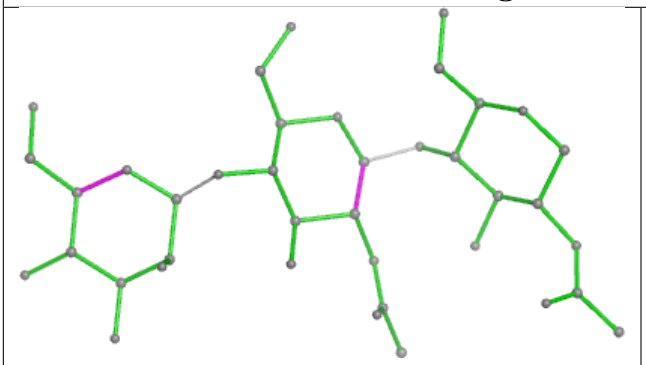


Torsions

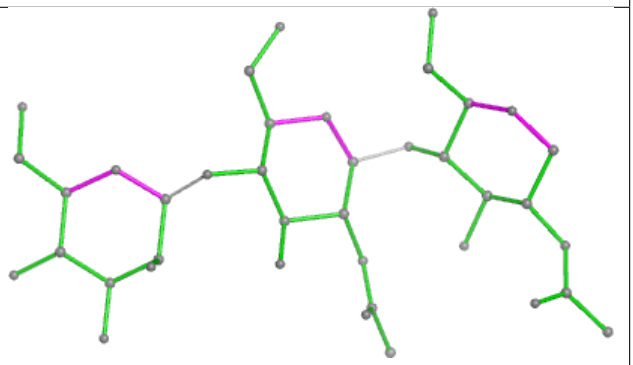


Rings

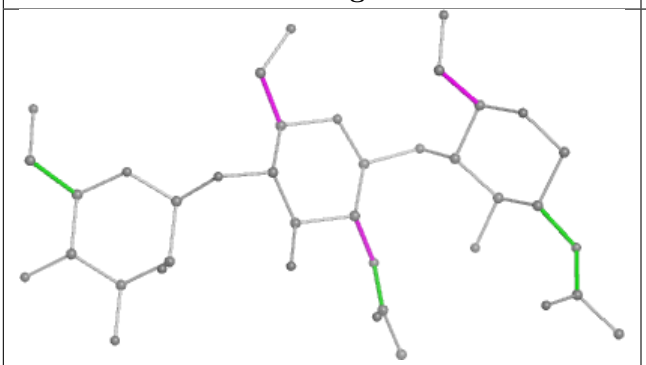
Oligosaccharide Chain L



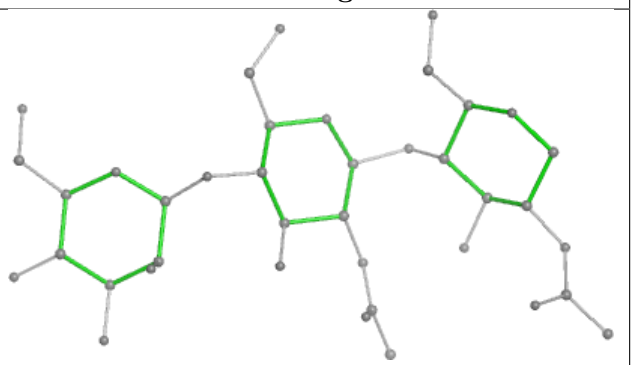
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

2 ligands 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	$\#\|Z\| > 2$
5	NAG	B	1077	1	14,14,15	0.31	0	17,19,21	0.39	0
5	NAG	F	1077	1	14,14,15	0.25	0	17,19,21	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1077	1	-	0/6/23/26	0/1/1/1
5	NAG	F	1077	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	460/539 (85%)	-0.41	6 (1%) 74 60	75, 111, 163, 220	0
1	B	458/539 (84%)	-0.45	0 100 100	81, 140, 212, 247	0
1	E	462/539 (85%)	-0.41	1 (0%) 92 87	65, 118, 173, 212	0
1	F	463/539 (85%)	-0.41	4 (0%) 81 68	67, 109, 158, 252	0
2	C	103/126 (81%)	-0.23	0 100 100	99, 146, 212, 291	0
2	D	104/126 (82%)	-0.47	0 100 100	110, 180, 237, 288	0
2	G	103/126 (81%)	-0.39	0 100 100	91, 165, 231, 258	0
2	H	104/126 (82%)	-0.48	0 100 100	74, 135, 217, 247	0
All	All	2257/2660 (84%)	-0.41	11 (0%) 87 78	65, 123, 204, 291	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	46	MET	4.1
1	A	357	LEU	2.5
1	A	97	LEU	2.5
1	F	403	LEU	2.4
1	A	81	LEU	2.3
1	A	485	CYS	2.3
1	F	470	VAL	2.3
1	A	379	ILE	2.1
1	A	121	LEU	2.1
1	F	31	LEU	2.1
1	E	46	MET	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

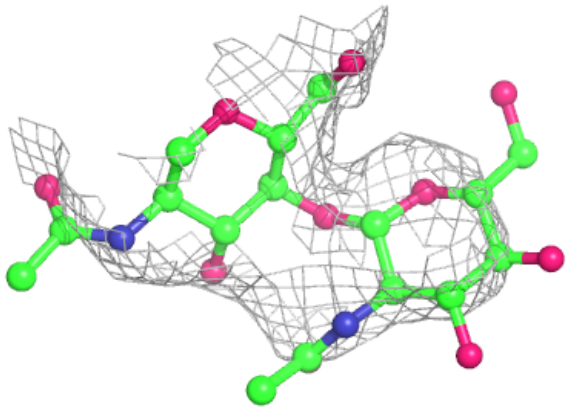
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

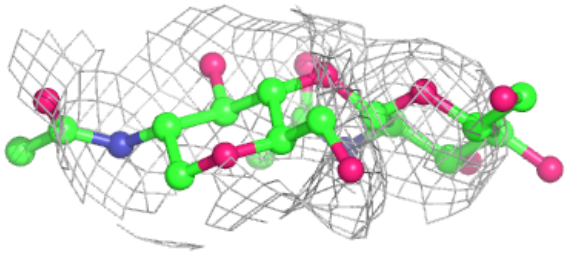
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	J	2	14/15	0.17	0.11	196,208,220,222	0
4	BMA	L	3	11/12	0.30	0.10	169,183,198,200	0
4	NAG	J	1	14/15	0.39	0.12	124,157,182,183	0
4	BMA	K	3	11/12	0.48	0.10	146,179,203,205	0
4	BMA	J	3	11/12	0.50	0.08	216,222,226,228	0
4	NAG	L	2	14/15	0.52	0.09	182,194,202,205	0
3	NAG	I	2	14/15	0.55	0.07	209,218,221,223	0
3	NAG	I	1	14/15	0.69	0.07	183,197,210,211	0
4	NAG	L	1	14/15	0.69	0.08	113,137,179,189	0
4	NAG	K	2	14/15	0.81	0.07	134,155,165,172	0
4	NAG	K	1	14/15	0.85	0.09	106,149,169,170	0

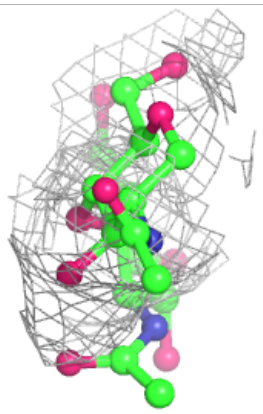
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

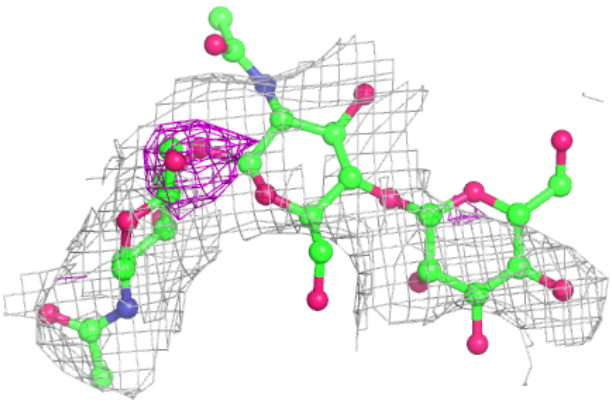


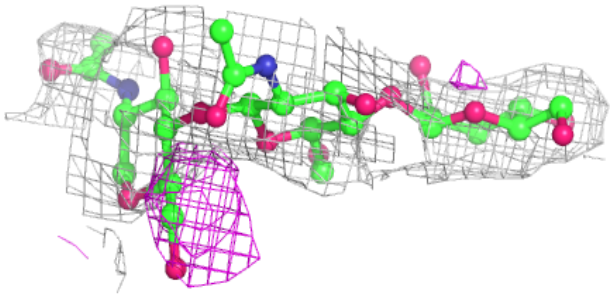


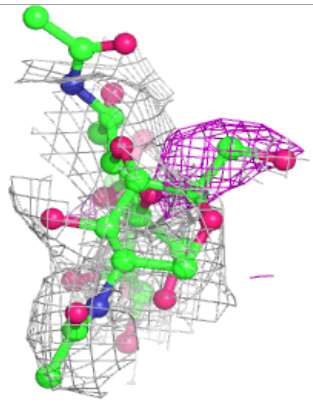


Electron density around Chain J:

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

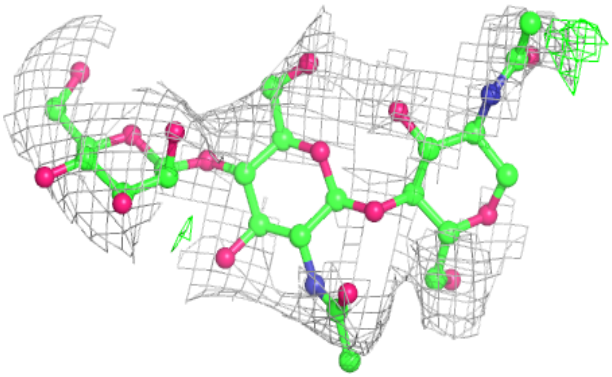


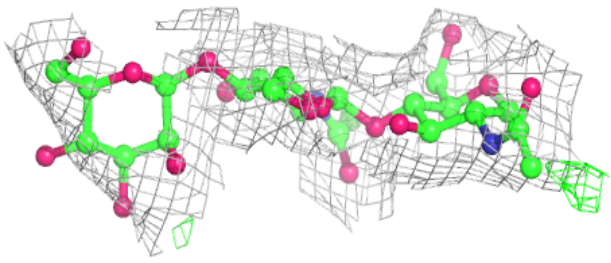


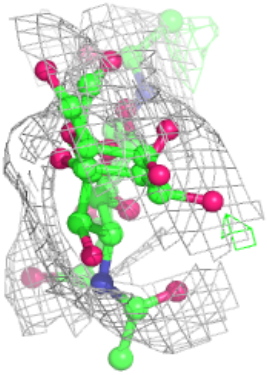


Electron density around Chain K:

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

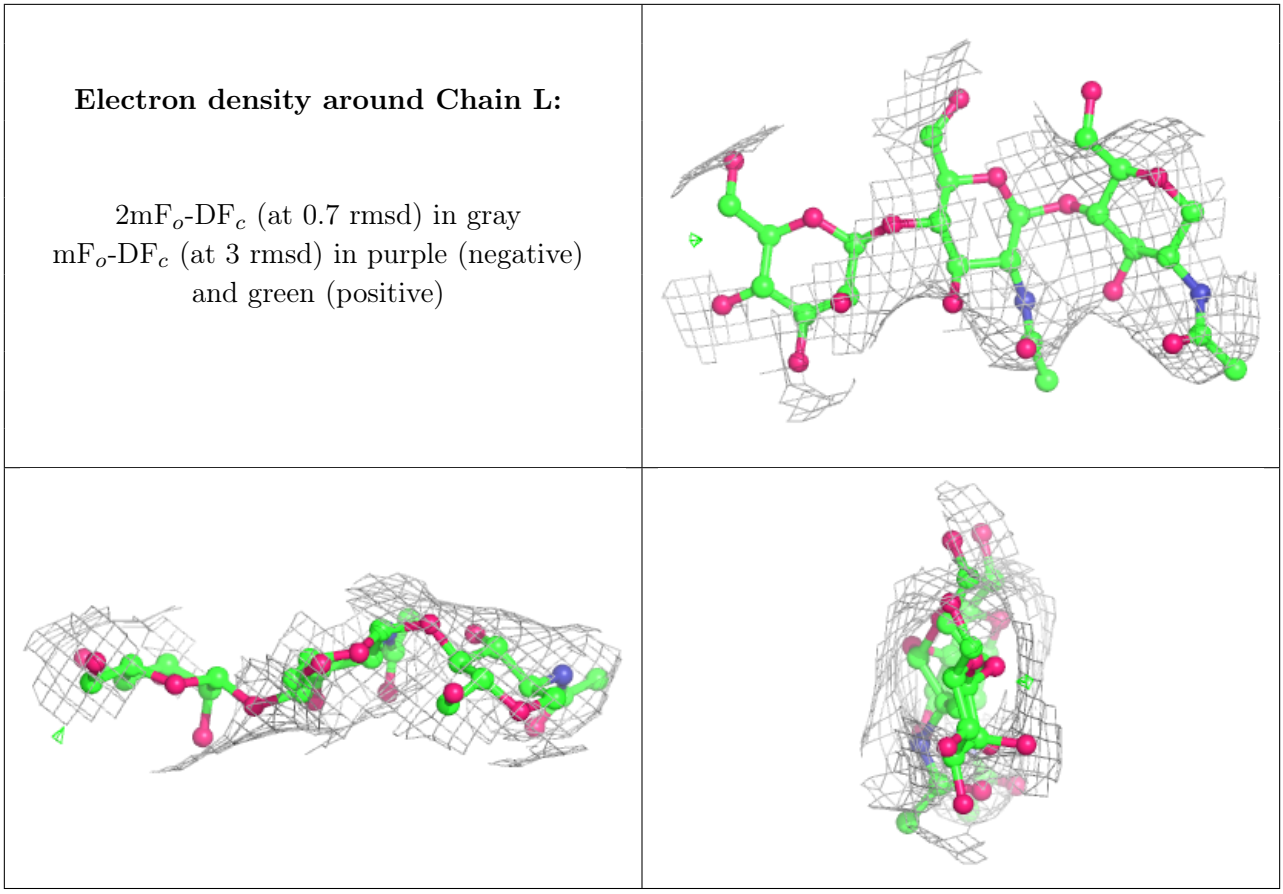






Electron density around Chain L:

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



6.4 Ligands

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, 95^{th} 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
5	NAG	B	1077	14/15	0.45	0.09	144,180,196,201	0
5	NAG	F	1077	14/15	0.58	0.07	169,175,193,196	0

6.5 Other polymers

There are no such residues in this entry.