Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2024 – 10:04 AM EDT

PDB ID	:	1G1S
Title	:	P-SELECTIN LECTIN/EGF DOMAINS COMPLEXED WITH PSGL-1 PEPTIDE
Authors	:	Somers, W.S.; Camphausen, R.T.
Deposited on	:	2000-10-13
Resolution	:	1.90 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:

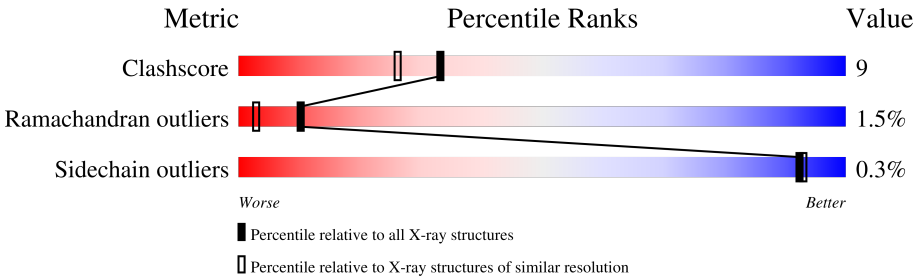
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	162	80% 16%
1	B	162	83% 12%
2	C	28	32% 14% 54%
2	D	28	43% 7% 50%
3	E	6	83% 17%
3	F	6	17% 83%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NGA	E	1	X	-	-	-
3	NGA	F	1	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 3258 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 P-SELECTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1292	817	217	247	11			
1	B	157	Total	C	N	O	S	0	0	0
			1275	808	212	245	10			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	ASP	GLU	conflict	UNP P16109
A	159	ASP	-	cloning artifact	UNP P16109
A	160	ASP	-	cloning artifact	UNP P16109
A	161	ASP	-	cloning artifact	UNP P16109
A	162	LYS	-	cloning artifact	UNP P16109
B	158	ASP	GLU	conflict	UNP P16109
B	159	ASP	-	cloning artifact	UNP P16109
B	160	ASP	-	cloning artifact	UNP P16109
B	161	ASP	-	cloning artifact	UNP P16109
B	162	LYS	-	cloning artifact	UNP P16109

- Molecule 2 is a protein called PSGL-1 PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	S	0	0	0
			119	74	13	30	2			
2	D	14	Total	C	N	O	S	0	0	0
			128	79	14	33	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	605	TYS	TYR	modified residue	UNP Q14242
C	607	TYS	TYR	modified residue	UNP Q14242

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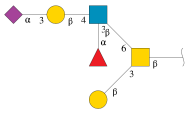
Chain	Residue	Modelled	Actual	Comment	Reference
C	610	TYS	TYR	modified residue	UNP Q14242
C	620	ARG	-	cloning artifact	UNP Q14242
C	621	PRO	-	cloning artifact	UNP Q14242
C	622	MET	-	cloning artifact	UNP Q14242
C	623	MET	-	cloning artifact	UNP Q14242
C	624	ASP	-	cloning artifact	UNP Q14242
C	625	ASP	-	cloning artifact	UNP Q14242
C	626	ASP	-	cloning artifact	UNP Q14242
C	627	ASP	-	cloning artifact	UNP Q14242
C	628	LYS	-	cloning artifact	UNP Q14242
D	605	TYS	TYR	modified residue	UNP Q14242
D	607	TYS	TYR	modified residue	UNP Q14242
D	610	TYS	TYR	modified residue	UNP Q14242
D	620	ARG	-	cloning artifact	UNP Q14242
D	621	PRO	-	cloning artifact	UNP Q14242
D	622	MET	-	cloning artifact	UNP Q14242
D	623	MET	-	cloning artifact	UNP Q14242
D	624	ASP	-	cloning artifact	UNP Q14242
D	625	ASP	-	cloning artifact	UNP Q14242
D	626	ASP	-	cloning artifact	UNP Q14242
D	627	ASP	-	cloning artifact	UNP Q14242
D	628	LYS	-	cloning artifact	UNP Q14242

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-[beta-D-galactopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			80	45	3	32			
3	F	6	Total	C	N	O	0	0	0
			80	45	3	32			

- Molecule 4 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Sr	0	0
			1	1		

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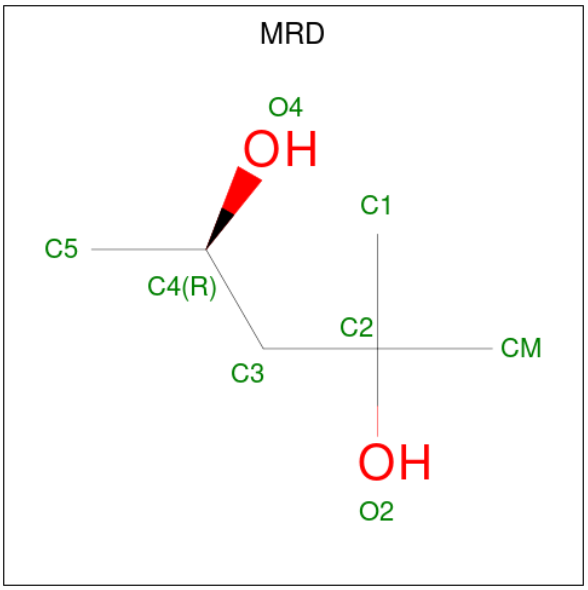
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Sr 1 1	0	0

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0
5	A	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0
5	B	1	Total C O 8 6 2	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Na 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	96	Total O 96 96	0	0
7	B	95	Total O 95 95	0	0
7	C	19	Total O 19 19	0	0
7	D	14	Total O 14 14	0	0

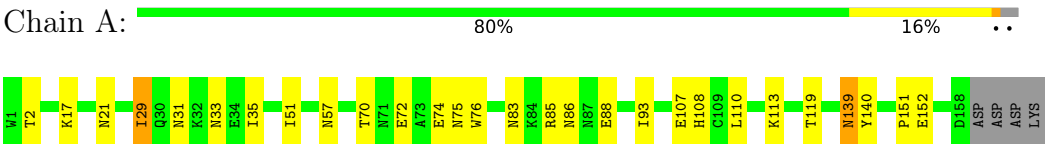
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

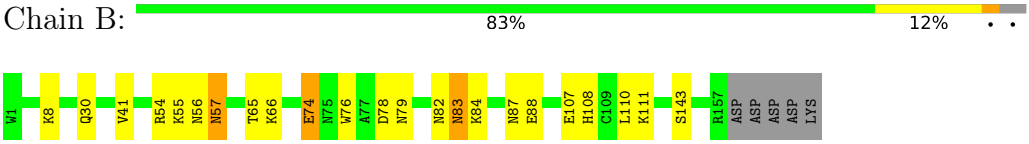
• Molecule 1: P-SELECTIN

Chain A:



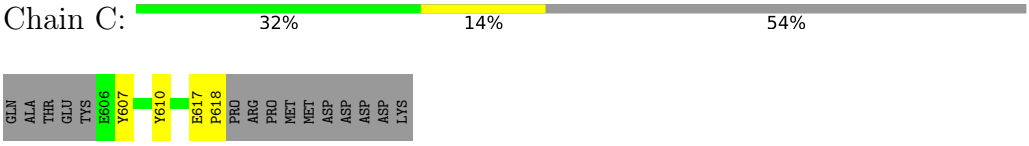
• Molecule 1: P-SELECTIN

Chain B:



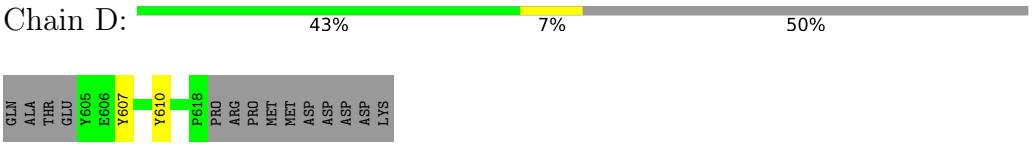
• Molecule 2: PSGL-1 PEPTIDE

Chain C:



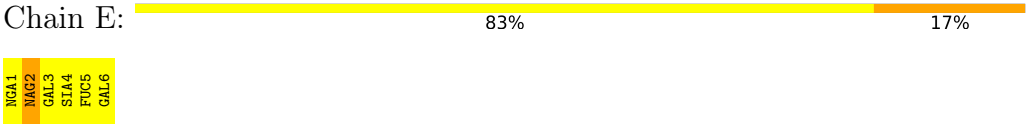
• Molecule 2: PSGL-1 PEPTIDE

Chain D:



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-[beta-D-galactopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose

Chain E:



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-[beta-D-galactopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-galactopyranose

Chain F:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	63.45Å 96.76Å 187.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-1.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3258	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, NGA, NA, FUC, GAL, MRD, SR, TYS, 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	0.48	0/1331	0.72	0/1811
1	B	0.46	0/1314	0.68	0/1790
2	C	0.36	0/87	0.63	0/116
2	D	0.46	0/91	0.71	0/121
All	All	0.47	0/2823	0.70	0/3838

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1292	0	1183	28	0
1	B	1275	0	1163	20	0
2	C	119	0	89	2	0
2	D	128	0	97	0	0
3	E	80	0	66	1	0
3	F	80	0	67	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	16	0	28	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	40	0	70	4	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	96	0	0	0	0
7	B	95	0	0	3	1
7	C	19	0	0	0	0
7	D	14	0	0	0	0
All	All	3258	0	2763	50	1

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 9.

All (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:HIS:HD2	1:B:110:LEU:H	1.22	0.86
1:A:108:HIS:HD2	1:A:110:LEU:H	1.23	0.85
1:A:139:ASN:HD21	5:A:811:MRD:H3C2	1.44	0.82
2:C:617:GLU:HB3	2:C:618:PRO:HD2	1.61	0.82
1:A:29:ILE:HD13	1:A:93:ILE:HD12	1.65	0.77
1:B:84:LYS:HG2	3:E:2:NAG:H83	1.66	0.74
1:B:83:ASN:ND2	1:B:88:GLU:H	1.87	0.73
1:B:41:VAL:HG21	5:B:806:MRD:H1C1	1.71	0.72
1:A:83:ASN:ND2	1:A:88:GLU:H	1.89	0.70
2:C:617:GLU:HB3	2:C:618:PRO:CD	2.22	0.69
1:A:17:LYS:NZ	1:A:21:ASN:HD21	1.90	0.69
1:A:139:ASN:ND2	5:A:811:MRD:H3C2	2.06	0.68
1:B:8:LYS:HD2	7:B:928:HOH:O	1.95	0.67
1:A:29:ILE:CD1	1:A:93:ILE:HD12	2.26	0.64
1:A:108:HIS:CD2	1:A:110:LEU:H	2.11	0.64
1:A:17:LYS:HZ3	1:A:21:ASN:HD21	1.43	0.64
1:A:139:ASN:ND2	1:A:140:TYR:H	1.96	0.63
1:B:83:ASN:HD21	1:B:88:GLU:H	1.44	0.63
1:B:107:GLU:OE1	1:B:111:LYS:HE2	1.98	0.63
1:A:29:ILE:HD12	1:A:51:ILE:HD13	1.80	0.62
1:B:30:GLN:NE2	5:B:808:MRD:H1C2	2.15	0.61
1:A:85:ARG:O	1:A:86:ASN:HB2	2.00	0.61
1:A:74:GLU:HG3	1:A:76:TRP:HD1	1.65	0.60
1:B:74:GLU:HG2	1:B:76:TRP:CD1	2.38	0.58
1:A:74:GLU:CG	1:A:76:TRP:HD1	2.15	0.58
1:A:152:GLU:OE2	5:A:811:MRD:HMC3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ARG:HD3	7:B:944:HOH:O	2.05	0.56
1:A:74:GLU:HG2	1:A:76:TRP:CD1	2.40	0.55
1:A:74:GLU:CG	1:A:76:TRP:CD1	2.92	0.53
1:B:108:HIS:CD2	1:B:110:LEU:H	2.13	0.53
1:A:139:ASN:CG	1:A:140:TYR:H	2.12	0.51
1:B:54:ARG:HG2	1:B:55:LYS:N	2.26	0.50
1:A:83:ASN:HD21	1:A:88:GLU:H	1.58	0.49
1:B:78:ASP:O	1:B:79:ASN:HB2	2.15	0.47
1:A:29:ILE:HD12	1:A:51:ILE:CD1	2.45	0.46
1:A:70:THR:OG1	1:A:72:GLU:HG2	2.17	0.45
1:B:83:ASN:HD21	1:B:87:ASN:N	2.15	0.45
1:A:29:ILE:O	1:A:29:ILE:HG22	2.16	0.44
1:B:108:HIS:HE1	7:B:922:HOH:O	1.99	0.44
1:B:56:ASN:O	1:B:57:ASN:CB	2.66	0.43
1:A:29:ILE:HD11	1:A:51:ILE:HG21	2.01	0.43
1:A:2:THR:HB	1:A:119:THR:HG22	1.99	0.43
1:A:35:ILE:HD13	1:A:75:ASN:ND2	2.33	0.42
1:B:65:THR:O	1:B:66:LYS:HB2	2.20	0.41
1:B:41:VAL:HG22	5:B:806:MRD:H3C2	2.02	0.41
1:A:31:ASN:OD1	1:A:33:ASN:HB2	2.20	0.41
1:B:82:ASN:O	1:B:83:ASN:C	2.59	0.41
1:B:143:SER:OG	5:B:809:MRD:H4	2.20	0.41
1:A:107:GLU:HG3	1:A:113:LYS:HE3	2.04	0.40
1:A:151:PRO:HB2	5:A:811:MRD:H1C2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:950:HOH:O	7:B:950:HOH:O[4_576]	1.88	0.32

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	156/162 (96%)	144 (92%)	9 (6%)	3 (2%)	8 1
1	B	155/162 (96%)	143 (92%)	10 (6%)	2 (1%)	12 4
2	C	9/28 (32%)	8 (89%)	1 (11%)	0	100 100
2	D	10/28 (36%)	9 (90%)	1 (10%)	0	100 100
All	All	330/380 (87%)	304 (92%)	21 (6%)	5 (2%)	10 3

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
1	A	57	ASN
1	A	139	ASN
1	B	57	ASN
1	B	74	GLU

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	138/147 (94%)	138 (100%)	0	100 100
1	B	136/147 (92%)	135 (99%)	1 (1%)	84 84
2	C	10/24 (42%)	10 (100%)	0	100 100
2	D	11/24 (46%)	11 (100%)	0	100 100
All	All	295/342 (86%)	294 (100%)	1 (0%)	92 93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	83	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	30	GLN
1	A	83	ASN
1	A	108	HIS
1	A	123	GLN
1	A	139	ASN
1	B	71	ASN
1	B	83	ASN
1	B	108	HIS
1	B	123	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TYS	D	607	2	15,16,17	1.58	2 (13%)	18,22,24	0.88	1 (5%)
2	TYS	D	605	2	3,4,17	0.75	0	2,4,24	0.84	0
2	TYS	D	610	2	15,16,17	1.39	2 (13%)	18,22,24	0.95	1 (5%)
2	TYS	C	607	2	15,16,17	1.45	3 (20%)	18,22,24	1.00	3 (16%)
2	TYS	C	610	2	15,16,17	1.38	3 (20%)	18,22,24	0.96	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TYS	D	607	2	-	1/10/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TYS	D	605	2	-	0/0/2/13	-
2	TYS	D	610	2	-	3/10/11/13	0/1/1/1
2	TYS	C	607	2	-	0/10/11/13	0/1/1/1
2	TYS	C	610	2	-	1/10/11/13	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	607	TYS	CE1-CD1	3.19	1.44	1.38
2	C	607	TYS	OH-CZ	-2.64	1.38	1.42
2	C	607	TYS	CE1-CD1	2.56	1.43	1.38
2	D	610	TYS	CE1-CD1	2.35	1.43	1.38
2	D	610	TYS	CD1-CG	2.35	1.43	1.38
2	C	610	TYS	CE1-CD1	2.23	1.42	1.38
2	C	607	TYS	CD1-CG	2.16	1.43	1.38
2	D	607	TYS	CE2-CZ	2.10	1.42	1.38
2	C	610	TYS	CD1-CG	2.05	1.43	1.38
2	C	610	TYS	CE2-CD2	2.01	1.42	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	610	TYS	O3-S-OH	2.43	111.69	105.83
2	C	610	TYS	O3-S-OH	2.39	111.59	105.83
2	D	607	TYS	O3-S-OH	2.37	111.53	105.83
2	C	607	TYS	O3-S-OH	2.20	111.12	105.83
2	C	607	TYS	CG-CB-CA	-2.05	109.95	114.10
2	C	607	TYS	CB-CA-C	-2.00	107.71	111.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	610	TYS	O-C-CA-CB
2	D	607	TYS	O-C-CA-CB
2	D	610	TYS	O-C-CA-CB
2	D	610	TYS	CA-CB-CG-CD1
2	D	610	TYS	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

12 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	NGA	E	1	2,3	14,14,15	0.80	0	17,19,21	1.19	2 (11%)
3	NAG	E	2	3	14,14,15	0.92	0	17,19,21	1.18	1 (5%)
3	GAL	E	3	3	11,11,12	0.60	0	15,15,17	1.10	1 (6%)
3	SIA	E	4	3	20,20,21	2.13	3 (15%)	24,28,31	1.49	6 (25%)
3	FUC	E	5	4,3	10,10,11	1.13	1 (10%)	14,14,16	1.13	2 (14%)
3	GAL	E	6	3	11,11,12	1.06	1 (9%)	15,15,17	1.36	3 (20%)
3	NGA	F	1	2,3	14,14,15	0.94	0	17,19,21	1.17	2 (11%)
3	NAG	F	2	3	14,14,15	0.79	0	17,19,21	1.10	1 (5%)
3	GAL	F	3	3	11,11,12	0.75	0	15,15,17	0.94	0
3	SIA	F	4	3	20,20,21	2.11	3 (15%)	24,28,31	1.47	4 (16%)
3	FUC	F	5	4,3	10,10,11	1.42	2 (20%)	14,14,16	0.98	1 (7%)
3	GAL	F	6	3	11,11,12	0.93	1 (9%)	15,15,17	1.34	4 (26%)

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	NGA	E	1	2,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	GAL	E	3	3	-	1/2/19/22	0/1/1/1
3	SIA	E	4	3	-	2/18/34/38	0/1/1/1
3	FUC	E	5	4,3	-	-	0/1/1/1
3	GAL	E	6	3	-	1/2/19/22	0/1/1/1
3	NGA	F	1	2,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	GAL	F	3	3	-	1/2/19/22	0/1/1/1
3	SIA	F	4	3	-	2/18/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	F	5	4,3	-	-	0/1/1/1
3	GAL	F	6	3	-	1/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	SIA	C2-C1	7.60	1.59	1.52
3	E	4	SIA	C2-C1	7.17	1.58	1.52
3	F	5	FUC	C2-C3	2.66	1.56	1.52
3	E	4	SIA	O1B-C1	-2.52	1.22	1.30
3	E	4	SIA	C3-C2	2.26	1.56	1.52
3	F	4	SIA	O1B-C1	-2.21	1.23	1.30
3	E	5	FUC	C4-C3	2.14	1.57	1.52
3	E	6	GAL	C4-C5	2.13	1.57	1.53
3	F	5	FUC	O5-C1	2.04	1.47	1.43
3	F	4	SIA	O4-C4	-2.04	1.39	1.43
3	F	6	GAL	C4-C5	2.03	1.57	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	4	SIA	C6-O6-C2	3.28	118.35	111.34
3	F	1	NGA	C1-O5-C5	3.03	116.30	112.19
3	E	4	SIA	C6-O6-C2	2.92	117.58	111.34
3	E	1	NGA	C1-O5-C5	2.79	115.98	112.19
3	E	6	GAL	O2-C2-C3	-2.64	104.86	110.14
3	E	4	SIA	O6-C2-C3	-2.57	106.92	110.46
3	E	6	GAL	C1-O5-C5	2.55	115.64	112.19
3	F	4	SIA	O1B-C1-C2	2.51	120.18	113.03
3	E	4	SIA	O1B-C1-C2	2.50	120.17	113.03
3	F	6	GAL	C1-O5-C5	2.37	115.40	112.19
3	E	5	FUC	C1-O5-C5	2.32	118.04	112.78
3	E	4	SIA	C5-N5-C10	2.24	128.63	123.18
3	F	6	GAL	O4-C4-C3	-2.22	105.22	110.35
3	F	4	SIA	O9-C9-C8	-2.21	106.25	111.07
3	E	2	NAG	O7-C7-N2	2.20	125.99	121.95
3	E	3	GAL	O2-C2-C3	-2.19	105.76	110.14
3	F	6	GAL	O2-C2-C3	-2.18	105.76	110.14
3	E	4	SIA	O6-C2-C1	2.14	111.91	107.70
3	E	5	FUC	O4-C4-C3	-2.14	105.39	110.35
3	F	2	NAG	O7-C7-N2	2.14	125.89	121.95
3	E	4	SIA	O9-C9-C8	-2.14	106.41	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1	NGA	O7-C7-N2	2.13	125.87	121.95
3	E	6	GAL	O4-C4-C3	-2.12	105.45	110.35
3	F	5	FUC	C1-O5-C5	2.09	117.51	112.78
3	F	4	SIA	O6-C2-C1	2.08	111.77	107.70
3	F	1	NGA	O7-C7-N2	2.03	125.68	121.95
3	F	6	GAL	O2-C2-C1	2.01	113.27	109.15

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	1	NGA	C1
3	F	1	NGA	C1

All (8) torsion outliers are listed below:

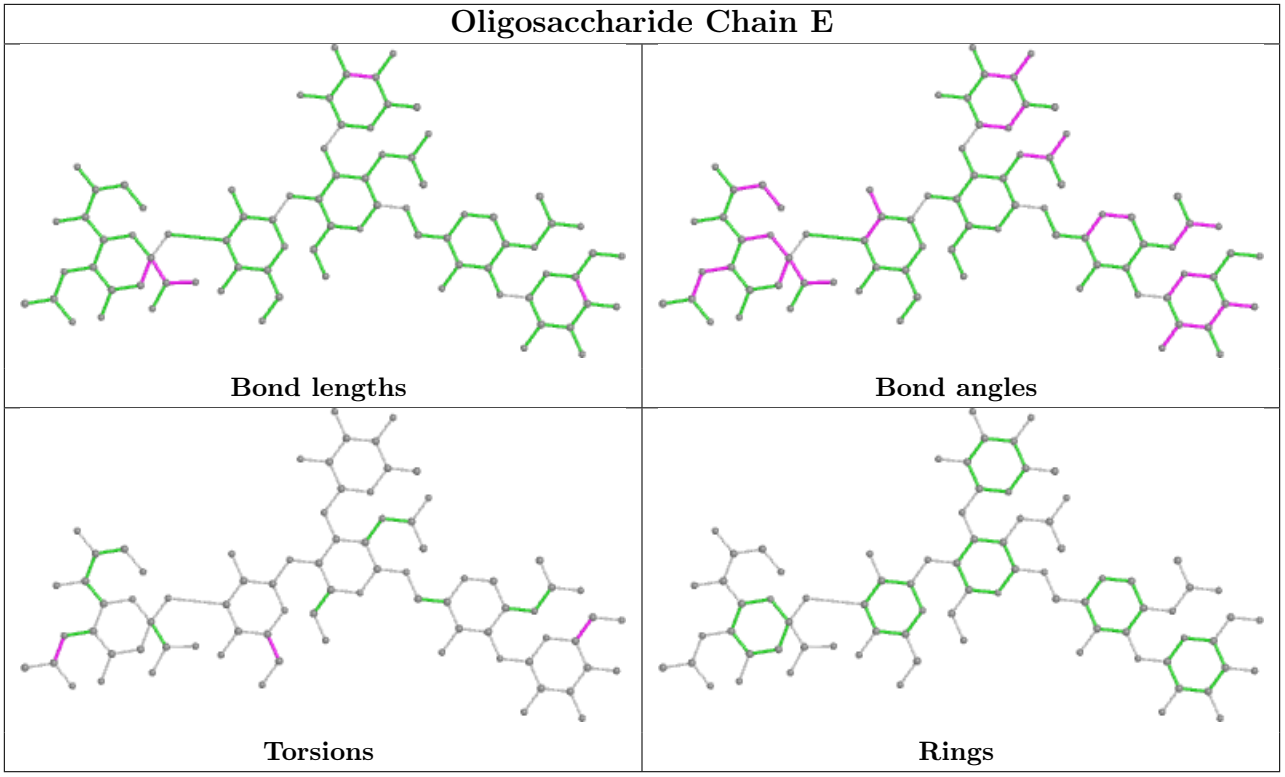
Mol	Chain	Res	Type	Atoms
3	E	4	SIA	C11-C10-N5-C5
3	E	4	SIA	O10-C10-N5-C5
3	F	4	SIA	C11-C10-N5-C5
3	F	4	SIA	O10-C10-N5-C5
3	E	3	GAL	O5-C5-C6-O6
3	E	6	GAL	O5-C5-C6-O6
3	F	6	GAL	O5-C5-C6-O6
3	F	3	GAL	O5-C5-C6-O6

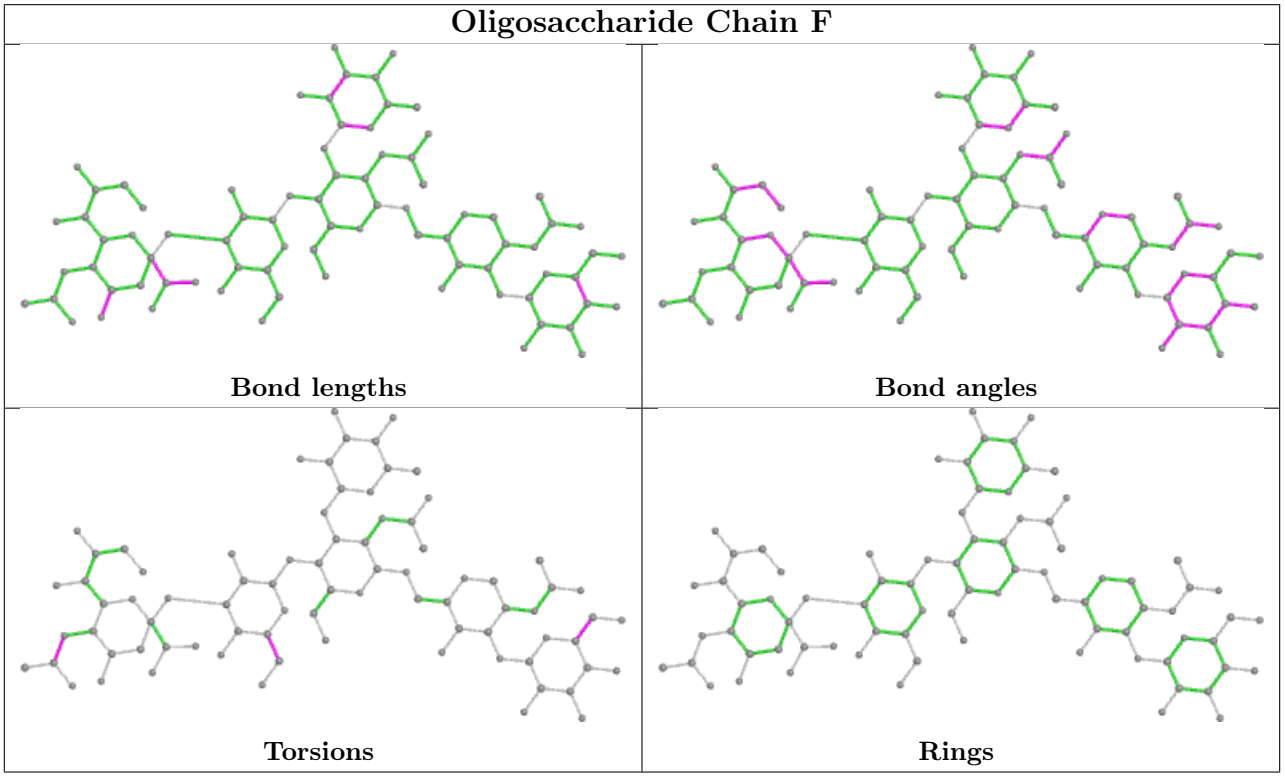
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	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.





5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	MRD	B	810	-	7,7,7	0.81	0	9,10,10	0.45	0
5	MRD	B	808	-	7,7,7	0.67	0	9,10,10	0.33	0
5	MRD	B	809	-	7,7,7	0.91	0	9,10,10	0.39	0
5	MRD	A	811	-	7,7,7	0.86	0	9,10,10	0.48	0
5	MRD	B	806	-	7,7,7	0.81	0	9,10,10	0.45	0
5	MRD	A	807	-	7,7,7	0.78	0	9,10,10	0.53	0
5	MRD	B	805	-	7,7,7	0.78	0	9,10,10	0.46	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	MRD	B	810	-	-	1/5/5/5	-
5	MRD	B	808	-	-	1/5/5/5	-
5	MRD	B	809	-	-	4/5/5/5	-
5	MRD	A	811	-	-	1/5/5/5	-
5	MRD	B	806	-	-	0/5/5/5	-
5	MRD	A	807	-	-	0/5/5/5	-
5	MRD	B	805	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	808	MRD	C2-C3-C4-O4
5	B	809	MRD	O2-C2-C3-C4
5	B	810	MRD	O2-C2-C3-C4
5	B	809	MRD	C1-C2-C3-C4
5	B	809	MRD	CM-C2-C3-C4
5	B	809	MRD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	A	811	MRD	C2-C3-C4-O4

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	808	MRD	1	0
5	B	809	MRD	1	0
5	A	811	MRD	4	0
5	B	806	MRD	2	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.