



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:31 PM GMT

PDB ID : 1G1R
Title : Crystal structure of P-selectin lectin/EGF domains complexed with SLeX
Authors : Somers, W.S.; Camphausen, R.T.
Deposited on : 2000-10-13
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

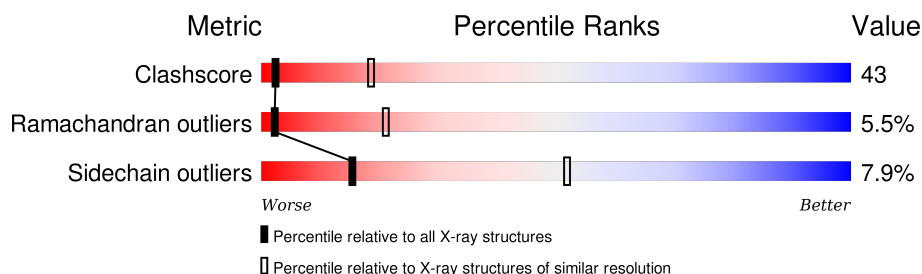
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

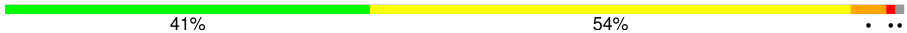



Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	162	
1	B	162	
1	C	162	
1	D	162	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5451 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	160	Total	C	N	O	S	0	0	0
			1315	829	222	253	11			
1	B	160	Total	C	N	O	S	0	0	0
			1319	832	223	253	11			
1	C	159	Total	C	N	O	S	0	0	0
			1307	825	220	251	11			
1	D	160	Total	C	N	O	S	0	0	0
			1319	832	223	253	11			

There are 20 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
C	158	ASP	GLU	CONFLICT	UNP P16109
C	159	ASP	-	cloning artifact	UNP P16109
C	160	ASP	-	cloning artifact	UNP P16109
C	161	ASP	-	cloning artifact	UNP P16109
C	162	LYS	-	cloning artifact	UNP P16109
D	158	ASP	GLU	CONFLICT	UNP P16109
D	159	ASP	-	cloning artifact	UNP P16109
D	160	ASP	-	cloning artifact	UNP P16109
D	161	ASP	-	cloning artifact	UNP P16109
D	162	LYS	-	cloning artifact	UNP P16109

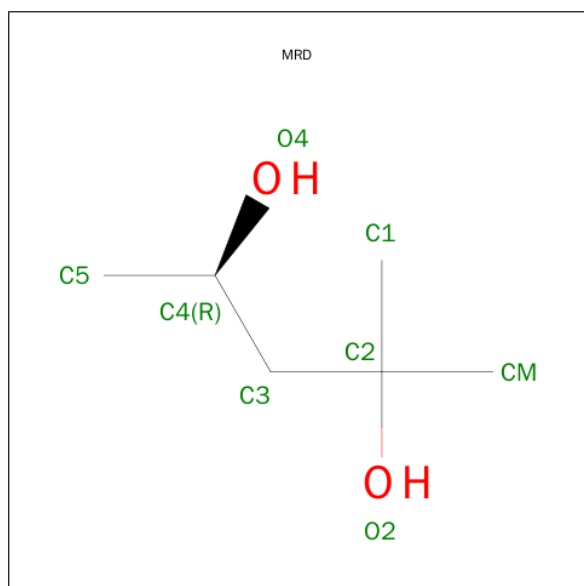
- Molecule 2 is a polymer of unknown type called SACCHARIDE (SIA-GAL-1NA-FUC).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			57	32	2	23		
2	B	4	Total	C	N	O	0	0
			57	32	2	23		
2	D	4	Total	C	N	O	0	0
			57	32	2	23		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			8	6	2		

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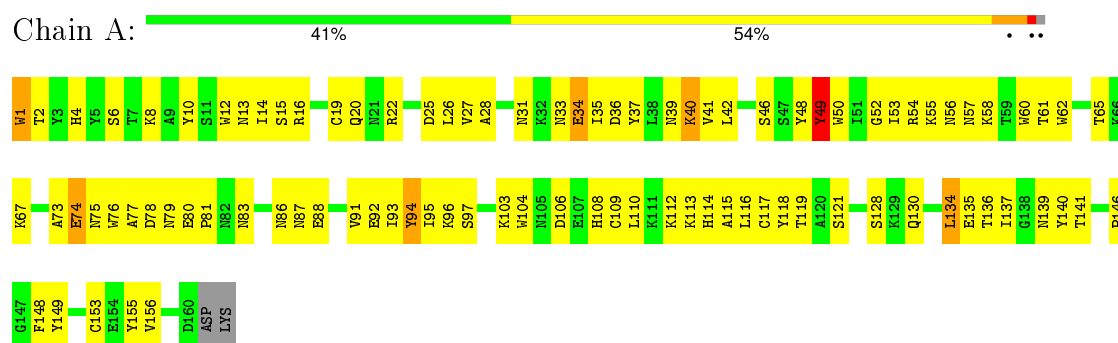
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	8	6	2	0	0

3 Residue-property plots

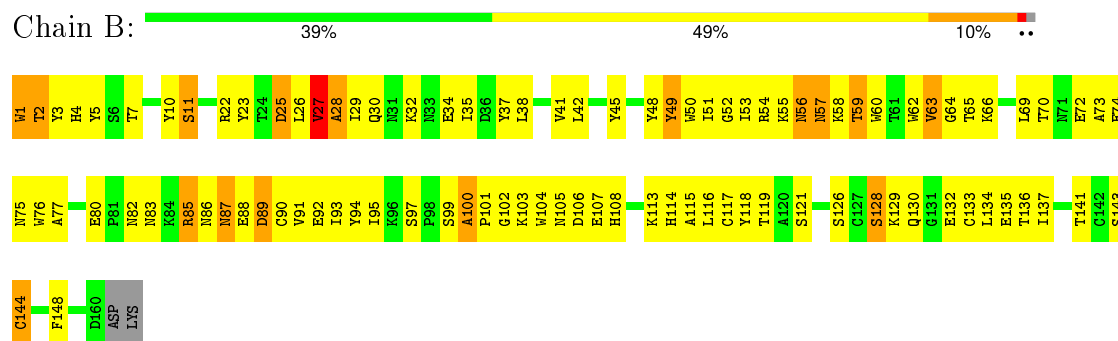
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

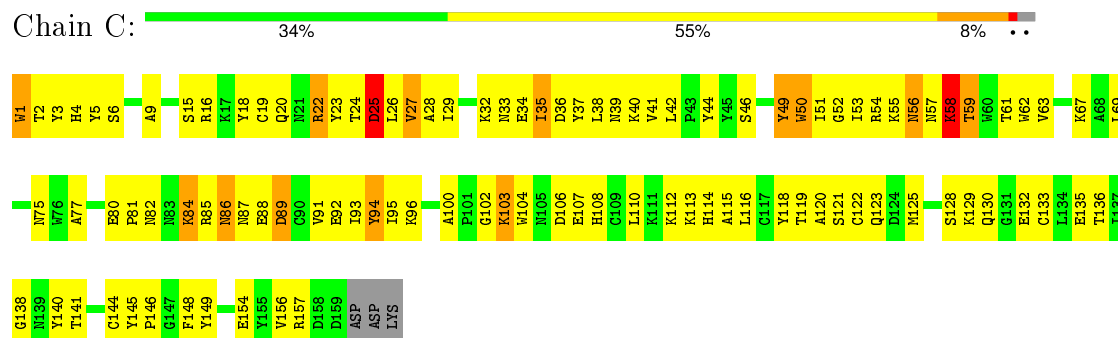
• Molecule 1: P-SELECTIN



• Molecule 1: P-SELECTIN

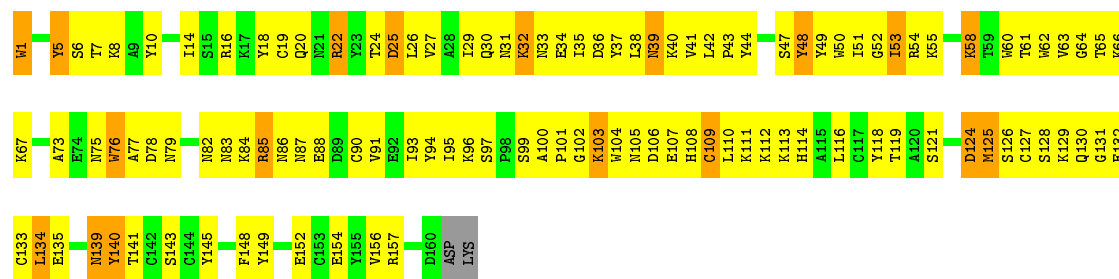


• Molecule 1: P-SELECTIN



- Molecule 1: P-SELECTIN

Chain D: 29% 59% 11%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.14Å 60.52Å 91.44Å 90.00° 103.28° 90.00°	Depositor
Resolution (Å)	14.00 – 3.40	Depositor
% Data completeness (in resolution range)	(Not available) (14.00-3.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.322	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5451	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SIA, GAL, FUC, MAG, MRD

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	0.58	0/1354	0.79	0/1841
1	B	0.47	0/1358	0.68	1/1845 (0.1%)
1	C	0.49	0/1346	0.72	0/1830
1	D	0.42	0/1358	0.67	0/1845
All	All	0.49	0/5416	0.71	1/7361 (0.0%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	28	ALA	N-CA-C	-5.25	96.83	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	49	TYR	Sidechain

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	1315	0	1208	98	0
1	B	1319	0	1219	108	0
1	C	1307	0	1202	112	0
1	D	1319	0	1219	138	0
2	A	57	0	52	0	0
2	B	57	0	51	4	0
2	D	57	0	51	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	8	0	14	0	0
4	C	8	0	14	0	0
All	All	5451	0	5030	450	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 43.

The worst 5 of 450 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:94:TYR:HB3	1:B:97:SER:HB2	1.35	1.09
1:C:77:ALA:HB2	1:C:103:LYS:HB3	1.41	1.00
1:B:77:ALA:HB3	1:B:80:GLU:HG3	1.43	0.99
1:B:27:VAL:HG21	1:B:116:LEU:HD23	1.47	0.97
1:A:86:ASN:H	1:D:130:GLN:HE21	1.07	0.96

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	158/162 (98%)	128 (81%)	26 (16%)	4 (2%)	7	43
1	B	158/162 (98%)	128 (81%)	20 (13%)	10 (6%)	2	18
1	C	157/162 (97%)	124 (79%)	24 (15%)	9 (6%)	2	20
1	D	158/162 (98%)	114 (72%)	32 (20%)	12 (8%)	1	13
All	All	631/648 (97%)	494 (78%)	102 (16%)	35 (6%)	2	21

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	CYS
1	B	11	SER
1	B	27	VAL
1	B	126	SER
1	B	144	CYS

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	142/147 (97%)	133 (94%)	9 (6%)	22	62
1	B	143/147 (97%)	131 (92%)	12 (8%)	14	49
1	C	141/147 (96%)	127 (90%)	14 (10%)	10	39
1	D	143/147 (97%)	133 (93%)	10 (7%)	19	58
All	All	569/588 (97%)	524 (92%)	45 (8%)	15	52

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	89	ASP
1	C	35	ILE

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Mol	Chain	Res	Type
1	D	103	LYS
1	C	22	ARG
1	C	49	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	105	ASN
1	C	75	ASN
1	D	123	GLN
1	C	56	ASN
1	C	79	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 ⓘ

12 carbohydrates 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	SIA	A	901	2	16,20,21	1.68	4 (25%)	18,28,31	1.25	1 (5%)
2	GAL	A	902	2	11,11,12	1.01	1 (9%)	14,15,17	1.26	2 (14%)
2	MAG	A	903	2	16,16,16	1.64	3 (18%)	21,22,22	1.74	3 (14%)
2	FUC	A	904	3,2	10,10,11	1.34	1 (10%)	14,14,16	1.45	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	B	901	2	16,20,21	1.39	3 (18%)	18,28,31	1.31	1 (5%)
2	GAL	B	902	2	11,11,12	1.11	1 (9%)	14,15,17	1.23	2 (14%)
2	MAG	B	903	2	16,16,16	1.44	2 (12%)	21,22,22	1.55	4 (19%)
2	FUC	B	904	3,2	10,10,11	0.95	0	14,14,16	1.14	1 (7%)
2	SIA	D	901	2	16,20,21	1.56	3 (18%)	18,28,31	1.32	2 (11%)
2	GAL	D	902	2	11,11,12	1.49	3 (27%)	14,15,17	1.35	3 (21%)
2	MAG	D	903	2	16,16,16	1.59	3 (18%)	21,22,22	1.34	3 (14%)
2	FUC	D	904	3,2	10,10,11	1.52	2 (20%)	14,14,16	1.21	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
2	SIA	A	901	2	-	0/14/34/38	0/1/1/1
2	GAL	A	902	2	-	0/2/19/22	0/1/1/1
2	MAG	A	903	2	-	1/8/28/28	0/1/1/1
2	FUC	A	904	3,2	-	0/0/17/20	0/1/1/1
2	SIA	B	901	2	-	0/14/34/38	0/1/1/1
2	GAL	B	902	2	-	0/2/19/22	0/1/1/1
2	MAG	B	903	2	-	1/8/28/28	0/1/1/1
2	FUC	B	904	3,2	-	0/0/17/20	0/1/1/1
2	SIA	D	901	2	-	0/14/34/38	0/1/1/1
2	GAL	D	902	2	-	0/2/19/22	0/1/1/1
2	MAG	D	903	2	-	0/8/28/28	0/1/1/1
2	FUC	D	904	3,2	-	0/0/17/20	0/1/1/1

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	903	MAG	C3-C2	2.05	1.57	1.53
2	D	904	FUC	C1-C2	2.05	1.57	1.52
2	D	902	GAL	C4-C5	2.07	1.57	1.53
2	A	902	GAL	C1-C2	2.10	1.57	1.52
2	D	901	SIA	C8-C7	2.11	1.57	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	SIA	C3-C4-C5	-3.60	107.47	111.47
2	B	903	MAG	C1-C2-N2	-2.46	106.38	111.01
2	D	902	GAL	O4-C4-C3	-2.37	105.00	110.34
2	D	903	MAG	C8-C7-N2	-2.30	111.70	116.11
2	D	901	SIA	C8-C7-C6	-2.29	108.41	113.01

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	903	MAG	CM-O1-C1-C2
2	A	903	MAG	CM-O1-C1-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	902	GAL	1	0
2	B	904	FUC	4	0
2	D	901	SIA	1	0

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
4	MRD	A	806	-	6,7,7	0.67	0	7,10,10	0.36	0
4	MRD	C	805	-	6,7,7	0.81	0	7,10,10	0.39	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
4	MRD	A	806	-	-	0/5/5/5	0/0/0/0
4	MRD	C	805	-	-	0/5/5/5	0/0/0/0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.