



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:12 PM GMT

PDB ID : 1SLT  
Title : STRUCTURE OF S-LECTIN, A DEVELOPMENTALLY REGULATED  
VERTEBRATE BETA-GALACTOSIDE BINDING PROTEIN  
Authors : Liao, D.-I.; Herzberg, O.  
Deposited on : 1993-10-20  
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](mailto: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.

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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

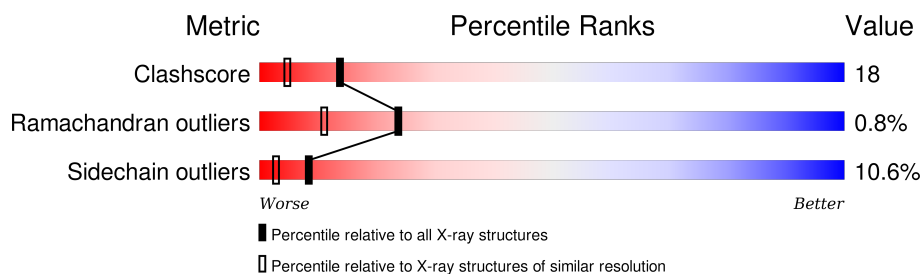
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	134	 49% 37% 12% ..
1	B	134	 59% 25% 13% ..

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2231 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 BOVINE GALECTIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1011	637	176	193	5			
1	B	132	Total	C	N	O	S	0	0	0
			1013	636	176	196	5			

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			26	14	1	11		
2	B	2	Total	C	N	O	0	0
			26	14	1	11		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

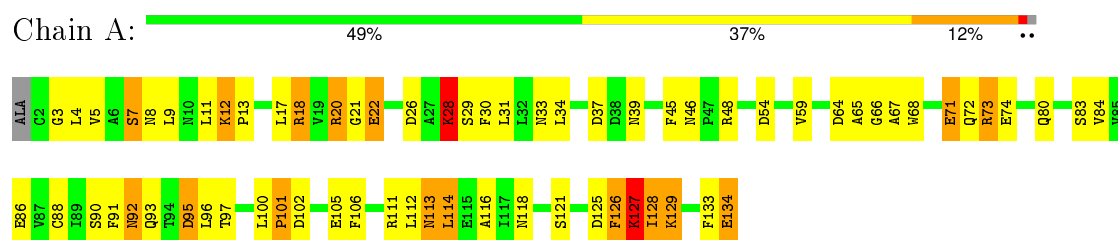
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	84	Total	O	0	0
			84	84		
4	B	70	Total	O	0	0
			70	70		

### 3 Residue-property plots [i](#)

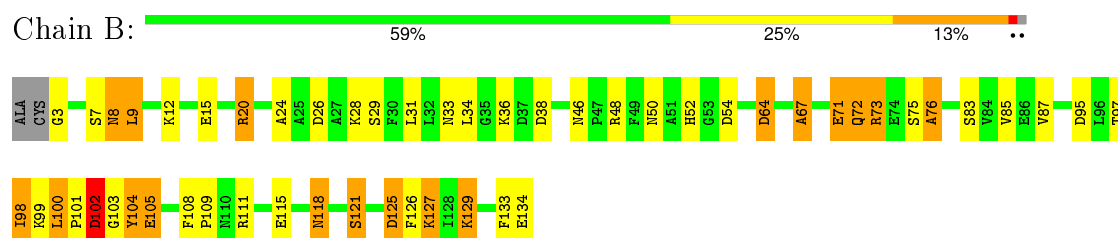
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: BOVINE GALECTIN-1



#### • Molecule 1: BOVINE GALECTIN-1



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.30 Å 62.90 Å 70.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, $R_{free}$	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2231	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	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: OCS, GAL, NDG, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.12	5/1006 (0.5%)	2.11	41/1354 (3.0%)
1	B	1.11	4/1008 (0.4%)	2.08	34/1357 (2.5%)
All	All	1.11	9/2014 (0.4%)	2.10	75/2711 (2.8%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	GLU	CD-OE1	6.71	1.33	1.25
1	A	22	GLU	CD-OE2	6.23	1.32	1.25
1	B	71	GLU	CD-OE1	6.04	1.32	1.25
1	A	71	GLU	CD-OE2	5.99	1.32	1.25
1	B	134	GLU	CD-OE1	5.88	1.32	1.25
1	B	115	GLU	CD-OE1	5.19	1.31	1.25
1	A	134	GLU	CD-OE1	5.14	1.31	1.25
1	A	105	GLU	CD-OE2	-5.04	1.20	1.25
1	A	86	GLU	CD-OE1	5.04	1.31	1.25

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ARG	NE-CZ-NH1	-12.46	114.07	120.30
1	B	38	ASP	CB-CG-OD2	-11.27	108.16	118.30
1	B	83	SER	N-CA-CB	-11.21	93.68	110.50
1	B	20	ARG	NE-CZ-NH2	-11.07	114.76	120.30
1	B	64	ASP	CB-CG-OD1	-10.69	108.68	118.30
1	B	125	ASP	CB-CG-OD2	10.48	127.74	118.30
1	B	38	ASP	CB-CG-OD1	10.27	127.54	118.30
1	B	125	ASP	CB-CG-OD1	-9.88	109.41	118.30
1	B	102	ASP	CB-CG-OD1	-9.73	109.54	118.30
1	B	64	ASP	CB-CG-OD2	9.57	126.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ASP	CB-CG-OD2	9.12	126.51	118.30
1	A	125	ASP	CB-CG-OD1	-8.77	110.41	118.30
1	A	114	LEU	CB-CA-C	-8.55	93.96	110.20
1	A	54	ASP	CB-CG-OD1	8.51	125.96	118.30
1	B	121	SER	N-CA-CB	8.49	123.24	110.50
1	A	37	ASP	CB-CG-OD1	8.38	125.84	118.30
1	A	102	ASP	CB-CG-OD2	-8.35	110.78	118.30
1	A	73	ARG	CD-NE-CZ	-8.27	112.02	123.60
1	A	121	SER	N-CA-CB	7.99	122.48	110.50
1	A	18	ARG	CB-CA-C	-7.88	94.65	110.40
1	A	20	ARG	CB-CA-C	-7.71	94.98	110.40
1	B	73	ARG	NE-CZ-NH1	-7.60	116.50	120.30
1	A	48	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	B	29	SER	N-CA-CB	-7.37	99.44	110.50
1	A	18	ARG	N-CA-CB	7.33	123.79	110.60
1	B	115	GLU	CA-CB-CG	-7.27	97.42	113.40
1	A	101	PRO	N-CA-CB	7.17	111.91	103.30
1	A	102	ASP	CB-CG-OD1	6.85	124.46	118.30
1	A	111	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	118	ASN	CA-CB-CG	-6.78	98.50	113.40
1	B	26	ASP	CB-CG-OD2	6.77	124.40	118.30
1	A	18	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	B	102	ASP	CB-CG-OD2	6.70	124.33	118.30
1	B	121	SER	CB-CA-C	-6.67	97.43	110.10
1	A	26	ASP	CB-CA-C	-6.58	97.24	110.40
1	B	95	ASP	CB-CG-OD1	6.53	124.18	118.30
1	A	65	ALA	N-CA-CB	6.40	119.06	110.10
1	A	4	LEU	CB-CA-C	-6.33	98.18	110.20
1	B	26	ASP	CB-CA-C	6.24	122.87	110.40
1	A	66	GLY	O-C-N	-6.19	112.80	122.70
1	B	52	HIS	C-N-CA	-6.18	109.31	122.30
1	A	126	PHE	N-CA-CB	-6.12	99.59	110.60
1	A	66	GLY	C-N-CA	-6.10	106.45	121.70
1	A	64	ASP	CB-CA-C	6.06	122.51	110.40
1	A	28	LYS	CB-CA-C	-5.96	98.47	110.40
1	B	111	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A	7	SER	N-CA-CB	5.91	119.36	110.50
1	A	26	ASP	N-CA-CB	-5.87	100.03	110.60
1	B	67	ALA	N-CA-CB	-5.86	101.90	110.10
1	A	46	ASN	N-CA-CB	-5.81	100.14	110.60
1	B	7	SER	CA-CB-OG	-5.79	95.57	111.20
1	A	3	GLY	N-CA-C	-5.73	98.77	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	67	ALA	CB-CA-C	-5.67	101.60	110.10
1	B	20	ARG	CG-CD-NE	-5.63	99.98	111.80
1	B	48	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	67	ALA	N-CA-CB	-5.50	102.40	110.10
1	A	127	LYS	CA-CB-CG	5.49	125.48	113.40
1	A	73	ARG	NH1-CZ-NH2	5.46	125.41	119.40
1	A	59	VAL	CA-CB-CG1	5.46	119.08	110.90
1	B	73	ARG	CD-NE-CZ	-5.42	116.01	123.60
1	A	95	ASP	N-CA-CB	-5.37	100.93	110.60
1	B	26	ASP	CA-CB-CG	5.35	125.17	113.40
1	B	8	ASN	CB-CG-OD1	-5.32	110.97	121.60
1	A	106	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	B	46	ASN	N-CA-CB	-5.29	101.08	110.60
1	A	64	ASP	N-CA-CB	5.29	120.11	110.60
1	A	114	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	A	29	SER	N-CA-CB	-5.22	102.67	110.50
1	A	39	ASN	CB-CA-C	-5.14	100.12	110.40
1	A	105	GLU	CB-CA-C	-5.13	100.14	110.40
1	A	111	ARG	CD-NE-CZ	5.12	130.76	123.60
1	B	72	GLN	N-CA-C	-5.11	97.21	111.00
1	B	9	LEU	CB-CG-CD1	-5.04	102.44	111.00
1	B	76	ALA	CB-CA-C	-5.01	102.58	110.10

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	1011	0	963	42	0
1	B	1013	0	972	36	0
2	A	26	0	24	1	0
2	B	26	0	24	0	0
3	A	1	0	0	0	0
4	A	84	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	70	0	0	5	0
All	All	2231	0	1983	75	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 18.

All (75) 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:127:LYS:NZ	1:A:129:LYS:HD2	1.93	0.84
1:A:127:LYS:CE	1:A:129:LYS:HD2	2.10	0.81
1:A:127:LYS:HE3	1:A:129:LYS:HD2	1.61	0.81
1:B:100:LEU:HB3	1:B:101:PRO:HD2	1.66	0.78
1:B:3:GLY:N	4:B:459:HOH:O	2.21	0.72
1:B:72:GLN:HB2	4:B:471:HOH:O	1.91	0.69
1:B:71:GLU:OE1	1:B:73:ARG:NH1	2.25	0.69
1:A:22:GLU:HG2	1:A:84:VAL:HG22	1.75	0.67
1:A:71:GLU:OE1	1:A:73:ARG:NH1	2.28	0.66
1:A:5:VAL:HG23	1:B:8:ASN:HD22	1.61	0.65
1:A:34:LEU:HD12	1:A:34:LEU:N	2.13	0.63
1:B:98:ILE:HD12	1:B:98:ILE:N	2.15	0.61
1:B:85:VAL:CG2	1:B:126:PHE:HE1	2.15	0.59
1:A:12:LYS:HB2	1:A:13:PRO:HD2	1.82	0.59
1:B:73:ARG:HG3	1:B:73:ARG:HH11	1.69	0.57
1:A:22:GLU:CG	1:A:84:VAL:HG22	2.34	0.56
1:A:13:PRO:HD3	1:A:91:PHE:CE2	2.41	0.55
1:A:126:PHE:CE2	1:A:128:ILE:CD1	2.89	0.55
1:A:31:LEU:C	1:A:31:LEU:HD12	2.27	0.55
1:A:28:LYS:NZ	4:A:586:HOH:O	2.30	0.54
1:B:33:ASN:C	1:B:34:LEU:HD12	2.28	0.53
1:A:100:LEU:HB3	1:A:101:PRO:HD2	1.91	0.53
1:B:108:PHE:CD1	1:B:109:PRO:HD2	2.44	0.52
1:B:85:VAL:HG22	1:B:126:PHE:HE1	1.75	0.52
1:A:21:GLY:HA3	1:A:126:PHE:CZ	2.45	0.52
1:B:50:ASN:HA	1:B:54:ASP:O	2.09	0.51
1:B:102:ASP:N	1:B:102:ASP:OD1	2.44	0.51
1:A:127:LYS:HE3	1:A:129:LYS:CD	2.38	0.51
1:A:18:ARG:HG3	1:A:134:GLU:OE1	2.10	0.51
1:B:102:ASP:OD1	1:B:104:TYR:CB	2.60	0.50
1:A:90:SER:HB2	1:A:97:THR:HB	1.93	0.50
1:A:129:LYS:HE3	1:B:133:PHE:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HB3	1:B:101:PRO:CD	2.40	0.50
1:B:101:PRO:C	1:B:103:GLY:H	2.15	0.50
1:B:73:ARG:CG	1:B:73:ARG:HH11	2.23	0.50
1:B:118:ASN:HB3	4:B:436:HOH:O	2.11	0.49
1:A:112:LEU:O	1:A:113:ASN:HB2	2.10	0.49
1:A:12:LYS:CB	1:A:13:PRO:HD2	2.44	0.48
1:A:92:ASN:ND2	1:A:95:ASP:O	2.46	0.48
1:A:33:ASN:C	1:A:34:LEU:HD12	2.33	0.48
1:B:64:ASP:O	1:B:67:ALA:HB3	2.13	0.47
1:A:127:LYS:HZ1	1:A:129:LYS:HD2	1.75	0.47
1:A:18:ARG:NH2	4:A:523:HOH:O	2.48	0.47
1:B:12:LYS:O	1:B:15:GLU:HG3	2.15	0.47
1:B:31:LEU:HD12	1:B:31:LEU:C	2.35	0.47
1:A:30:PHE:HB2	1:A:126:PHE:HB2	1.98	0.46
1:A:126:PHE:CE2	1:A:128:ILE:HD12	2.50	0.46
1:A:12:LYS:HB3	1:A:12:LYS:HE3	1.33	0.46
1:A:31:LEU:HA	1:A:45:PHE:O	2.16	0.45
1:A:18:ARG:HG2	1:A:88:OCS:SG	2.57	0.45
1:A:80:GLN:O	1:A:83:SER:OG	2.21	0.45
1:A:93:GLN:O	4:A:521:HOH:O	2.21	0.45
1:B:129:LYS:HD2	1:B:129:LYS:HA	1.54	0.44
1:A:112:LEU:HD23	1:A:114:LEU:HD21	1.99	0.44
1:A:12:LYS:HB2	1:A:13:PRO:CD	2.47	0.44
1:B:125:ASP:HA	4:B:480:HOH:O	2.18	0.43
1:B:28:LYS:HB3	1:B:28:LYS:HE3	1.54	0.43
1:A:12:LYS:CB	1:A:13:PRO:CD	2.96	0.43
1:B:73:ARG:CG	1:B:73:ARG:NH1	2.81	0.43
1:B:100:LEU:CB	1:B:101:PRO:CD	2.96	0.43
1:A:91:PHE:HE2	1:A:116:ALA:HA	1.83	0.42
1:B:67:ALA:O	4:B:429:HOH:O	2.21	0.42
1:A:129:LYS:CE	1:B:133:PHE:O	2.67	0.42
1:B:24:ALA:HB3	1:B:125:ASP:HB3	2.02	0.42
1:B:127:LYS:HG3	1:B:127:LYS:O	2.20	0.41
1:B:97:THR:HG21	1:B:99:LYS:HE3	2.02	0.41
1:B:101:PRO:C	1:B:103:GLY:N	2.73	0.41
1:A:68:TRP:CZ2	2:A:402:GAL:H4	2.56	0.41
1:B:75:SER:O	1:B:76:ALA:C	2.57	0.41
1:A:9:LEU:O	1:A:118:ASN:ND2	2.33	0.41
1:A:133:PHE:O	1:A:134:GLU:HG3	2.20	0.40
1:B:97:THR:CG2	1:B:99:LYS:HE3	2.51	0.40
1:B:133:PHE:CD1	1:B:133:PHE:N	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:SER:HB2	1:A:8:ASN:H	1.72	0.40
1:A:72:GLN:NE2	4:A:552:HOH:O	2.47	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	128/134 (96%)	124 (97%)	4 (3%)	0	100	100
1	B	127/134 (95%)	119 (94%)	6 (5%)	2 (2%)	12	3
All	All	255/268 (95%)	243 (95%)	10 (4%)	2 (1%)	24	11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	104	TYR
1	B	102	ASP

### 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	102/107 (95%)	90 (88%)	12 (12%)	6	2
1	B	105/107 (98%)	95 (90%)	10 (10%)	11	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	207/214 (97%)	185 (89%)	22 (11%)	<b>8</b> <b>3</b>

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	12	LYS
1	A	17	LEU
1	A	20	ARG
1	A	28	LYS
1	A	74	GLU
1	A	92	ASN
1	A	96	LEU
1	A	113	ASN
1	A	127	LYS
1	A	128	ILE
1	A	129	LYS
1	B	9	LEU
1	B	20	ARG
1	B	36	LYS
1	B	87	VAL
1	B	98	ILE
1	B	100	LEU
1	B	105	GLU
1	B	121	SER
1	B	127	LYS
1	B	129	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	B	8	ASN
1	B	56	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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
1	OCS	A	130	1	3,6,9	0.73	0	3,6,13	2.48	2 (66%)
1	OCS	A	16	1	3,7,9	0.78	0	3,8,13	3.84	3 (100%)
1	OCS	A	88	1	3,7,9	0.70	0	3,8,13	2.73	2 (66%)
1	OCS	B	130	1	3,6,9	0.98	0	3,6,13	1.71	0
1	OCS	B	16	1	3,7,9	1.09	0	3,8,13	4.90	2 (66%)
1	OCS	B	88	1	3,6,9	0.76	0	3,6,13	1.86	1 (33%)

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
1	OCS	A	130	1	-	0/1/5/9	0/0/0/0
1	OCS	A	16	1	-	0/2/6/9	0/0/0/0
1	OCS	A	88	1	-	0/2/6/9	0/0/0/0
1	OCS	B	130	1	-	0/1/5/9	0/0/0/0
1	OCS	B	16	1	-	1/2/6/9	0/0/0/0
1	OCS	B	88	1	-	0/1/5/9	0/0/0/0

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	OCS	OD1-SG-CB	-5.84	95.67	105.40
1	A	88	OCS	O-C-CA	-3.43	116.55	125.49
1	A	130	OCS	O-C-CA	-3.26	117.00	125.49
1	B	16	OCS	O-C-CA	-2.85	118.06	125.49
1	B	88	OCS	O-C-CA	-2.57	118.79	125.49
1	A	130	OCS	CB-CA-C	-2.57	104.42	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	OCS	O-C-CA	-2.30	119.51	125.49
1	A	16	OCS	CB-CA-C	-2.19	105.47	111.46
1	A	88	OCS	OD1-SG-CB	2.72	109.93	105.40
1	B	16	OCS	OD1-SG-CB	7.99	118.72	105.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	16	OCS	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	88	OCS	1	0

## 5.5 Carbohydrates [i](#)

4 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	NDG	A	401	2	15,15,15	1.27	2 (13%)	17,21,21	1.26	2 (11%)
2	GAL	A	402	2	11,11,12	0.59	0	14,15,17	2.32	6 (42%)
2	NDG	B	411	2	15,15,15	0.97	1 (6%)	17,21,21	2.04	6 (35%)
2	GAL	B	412	2	11,11,12	1.35	1 (9%)	14,15,17	2.05	6 (42%)

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	NDG	A	401	2	-	0/6/26/26	0/1/1/1
2	GAL	A	402	2	-	0/2/19/22	0/1/1/1
2	NDG	B	411	2	-	0/6/26/26	0/1/1/1
2	GAL	B	412	2	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	411	NDG	O-C1	2.26	1.47	1.43
2	A	401	NDG	C3-C2	2.48	1.58	1.53
2	A	401	NDG	C1-C2	3.05	1.56	1.53
2	B	412	GAL	C2-C3	3.90	1.57	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	GAL	O5-C1-C2	-5.77	101.49	110.86
2	B	412	GAL	O5-C5-C6	-3.85	99.01	107.35
2	B	411	NDG	O7-C7-C8	-3.60	115.46	122.06
2	B	412	GAL	O2-C2-C1	-3.03	103.13	109.21
2	B	412	GAL	O6-C6-C5	-2.88	101.82	111.33
2	A	402	GAL	O4-C4-C3	-2.87	103.87	110.34
2	A	402	GAL	O3-C3-C2	-2.82	104.90	110.00
2	A	401	NDG	O1L-C1-O	-2.78	102.64	110.25
2	B	412	GAL	C3-C4-C5	-2.72	105.45	110.20
2	B	411	NDG	C2-N2-C7	-2.65	116.30	123.10
2	A	402	GAL	O3-C3-C4	-2.57	104.56	110.34
2	B	412	GAL	O5-C1-C2	-2.30	107.12	110.86
2	B	412	GAL	O3-C3-C2	-2.08	106.24	110.00
2	A	402	GAL	O5-C5-C6	-2.07	102.86	107.35
2	A	401	NDG	O3-C3-C2	2.09	113.91	109.66
2	B	411	NDG	C8-C7-N2	2.27	120.45	116.11
2	B	411	NDG	O3-C3-C4	2.52	116.01	110.34
2	A	402	GAL	C1-C2-C3	3.05	113.14	109.54
2	B	411	NDG	O-C5-C6	3.74	115.80	106.36
2	B	411	NDG	C4-C3-C2	4.38	116.50	110.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	GAL	1	0

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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