



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:23 AM GMT

PDB ID : 3EF2
Title : Structure of the Marasmius oreades mushroom lectin (MOA) in complex with Galalpha(1,3)[Fucalpha(1,2)]Gal and Calcium.
Authors : Grahn, E.M.; Goldstein, I.J.; Krenzel, U.
Deposited on : 2008-09-08
Resolution : 1.80 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
<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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

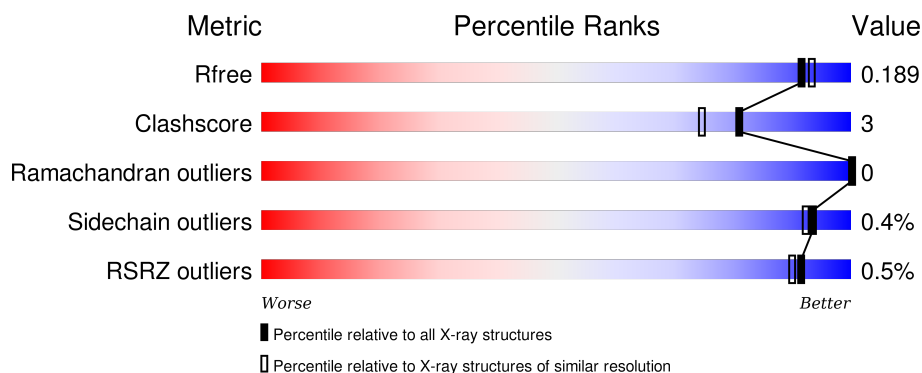
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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.

Mol	Chain	Length	Quality of chain
1	A	293	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
1	B	293	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
1	C	293	<div> <div></div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
1	D	293	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	A	306	-	-	X	X
5	ACT	A	309	-	-	-	X
5	ACT	C	306	-	-	X	X
5	ACT	D	304	-	-	X	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11033 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 Agglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	10	0
			2327	1488	381	449	9			
1	B	292	Total	C	N	O	S	0	11	0
			2336	1493	383	451	9			
1	C	292	Total	C	N	O	S	0	13	0
			2348	1501	385	453	9			
1	D	292	Total	C	N	O	S	0	12	0
			2336	1494	382	451	9			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	3	Total	C	O	0	0
			33	18	15		
2	A	3	Total	C	O	0	0
			33	18	15		
2	B	3	Total	C	O	0	0
			33	18	15		
2	B	3	Total	C	O	0	0
			33	18	15		
2	C	3	Total	C	O	0	0
			33	18	15		
2	C	3	Total	C	O	0	0
			33	18	15		
2	D	3	Total	C	O	0	0
			33	18	15		
2	D	3	Total	C	O	0	0
			33	18	15		

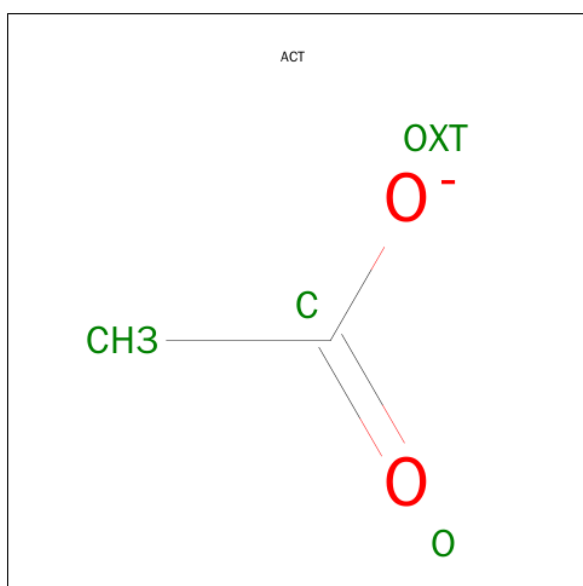
- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	3	Total	C	O	0	0
			33	18	15		
3	B	3	Total	C	O	0	0
			33	18	15		
3	C	3	Total	C	O	0	0
			33	18	15		
3	D	3	Total	C	O	0	0
			33	18	15		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Ca	0	0
			3	3		
4	A	5	Total	Ca	0	0
			5	5		
4	D	3	Total	Ca	0	0
			3	3		
4	C	5	Total	Ca	0	0
			5	5		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	327	Total	O	0	0
			327	327		
6	B	305	Total	O	0	1
			305	305		
6	C	315	Total	O	0	0
			315	315		
6	D	311	Total	O	0	0
			311	311		

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.

- Molecule 1: Agglutinin

Chain A: 



- Molecule 1: Agglutinin

Chain B: 



- Molecule 1: Agglutinin

Chain C: 



- Molecule 1: Agglutinin

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	121.28Å 121.28Å 100.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.80 46.51 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-1.80) 99.1 (46.51-1.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.165 , 0.189 0.164 , 0.189	Depositor DCC
R_{free} test set	7603 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	11.8	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.3	EDS
Estimated twinning fraction	0.487 for -h,-k,l 0.487 for h,-h-k,-l 0.487 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 151438 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11033	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: GLA, CA, GAL, FUC, ACT, OCS

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	0.63	0/2418	0.63	1/3292 (0.0%)
1	B	0.61	0/2427	0.64	0/3304
1	C	0.62	0/2442	0.63	0/3323
1	D	0.63	0/2433	0.63	1/3312 (0.0%)
All	All	0.62	0/9720	0.63	2/13231 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ASP	CB-CG-OD1	5.32	123.09	118.30
1	D	216	ASP	CB-CG-OD1	5.06	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2327	0	2189	15	0
1	B	2336	0	2196	13	0
1	C	2348	0	2213	14	0
1	D	2336	0	2202	17	0
2	A	66	0	60	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	66	0	60	0	0
2	C	66	0	60	0	0
2	D	66	0	60	0	0
3	A	33	0	30	0	0
3	B	33	0	30	0	0
3	C	33	0	30	0	0
3	D	33	0	30	0	0
4	A	5	0	0	0	0
4	B	3	0	0	0	0
4	C	5	0	0	0	0
4	D	3	0	0	0	0
5	A	8	0	6	3	0
5	C	4	0	3	2	0
5	D	4	0	3	4	0
6	A	327	0	0	9	0
6	B	305	0	0	8	0
6	C	315	0	0	7	0
6	D	311	0	0	10	0
All	All	11033	0	9172	62	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 3.

All (62) 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:D:199:LYS:HE3	6:D:491:HOH:O	1.77	0.83
1:A:216:ASP:O	1:A:220[B]:ILE:HG12	1.82	0.79
1:C:216:ASP:O	1:C:220[B]:ILE:HG12	1.82	0.78
1:A:139[A]:THR:HG22	6:A:451:HOH:O	1.89	0.71
1:A:199:LYS:HE3	6:A:608:HOH:O	1.91	0.70
1:B:172:HIS:HD2	6:B:780:HOH:O	1.76	0.68
1:D:276:GLN:O	6:D:485:HOH:O	2.10	0.68
1:B:139[B]:THR:HG22	6:B:643:HOH:O	1.95	0.67
1:B:276:GLN:O	6:B:760:HOH:O	2.12	0.66
1:A:172:HIS:HD2	6:A:461:HOH:O	1.77	0.66
1:C:139[B]:THR:HG22	6:C:718:HOH:O	1.97	0.65
1:D:216:ASP:HB3	5:D:304:ACT:H3	1.78	0.64
1:B:178:ARG:CZ	6:B:781:HOH:O	2.45	0.64
1:B:139[B]:THR:CG2	6:B:643:HOH:O	2.47	0.62
1:C:172:HIS:HD2	6:C:739:HOH:O	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:306:ACT:H3	6:A:539:HOH:O	1.98	0.62
1:A:55:ASN:ND2	1:C:55:ASN:OD1	2.33	0.61
1:C:38:THR:H	1:C:43:ASN:HD21	1.49	0.60
1:B:38:THR:H	1:B:43:ASN:HD21	1.49	0.60
1:D:38:THR:H	1:D:43:ASN:HD21	1.50	0.59
1:A:139[A]:THR:CG2	6:A:451:HOH:O	2.48	0.59
1:C:276:GLN:O	6:C:843:HOH:O	2.16	0.59
5:C:306:ACT:H2	6:C:794:HOH:O	2.03	0.59
1:D:216:ASP:O	1:D:220[B]:ILE:HG12	2.01	0.59
1:C:178:ARG:CZ	6:C:845:HOH:O	2.51	0.59
1:A:258:ALA:HB2	5:A:306:ACT:H2	1.83	0.58
1:B:216:ASP:O	1:B:220[B]:ILE:HG12	2.03	0.58
1:D:139[B]:THR:HG22	6:D:447:HOH:O	2.04	0.57
1:A:38:THR:H	1:A:43:ASN:HD21	1.51	0.57
1:B:7:ILE:HD13	1:B:65[A]:LEU:HD11	1.87	0.57
5:D:304:ACT:H2	6:D:530:HOH:O	2.03	0.57
1:C:139[B]:THR:CG2	6:C:718:HOH:O	2.52	0.55
1:A:276:GLN:O	6:A:556:HOH:O	2.18	0.55
1:D:216:ASP:HB3	5:D:304:ACT:CH3	2.39	0.53
1:A:7:ILE:HD13	1:A:65[A]:LEU:HD11	1.91	0.53
1:D:199:LYS:HE2	6:D:432:HOH:O	2.08	0.52
1:B:178:ARG:NH2	6:B:781:HOH:O	2.43	0.52
1:C:89:GLY:HA3	1:C:98:GLN:HE22	1.74	0.52
1:B:89:GLY:HA3	1:B:98:GLN:HE22	1.74	0.51
5:A:309:ACT:H2	6:B:722:HOH:O	2.09	0.51
1:C:178:ARG:NH2	6:C:845:HOH:O	2.44	0.50
1:D:89:GLY:HA3	1:D:98:GLN:HE22	1.76	0.49
1:A:172:HIS:HE1	6:A:548:HOH:O	1.95	0.48
1:A:89:GLY:HA3	1:A:98:GLN:HE22	1.78	0.48
1:A:199:LYS:HE2	6:A:435:HOH:O	2.13	0.48
1:D:7:ILE:HD13	1:D:65[A]:LEU:HD11	1.96	0.48
1:B:172:HIS:HE1	6:B:708:HOH:O	1.96	0.47
1:D:172:HIS:HD2	6:D:565:HOH:O	1.97	0.47
5:D:304:ACT:CH3	6:D:530:HOH:O	2.62	0.47
1:D:47:LEU:HD22	1:D:156[B]:MET:HG3	1.97	0.47
1:C:196:GLN:HE22	1:C:199[A]:LYS:NZ	2.14	0.45
1:C:7:ILE:HD13	1:C:65[A]:LEU:HD11	1.98	0.45
1:C:258:ALA:HB2	5:C:306:ACT:H1	1.97	0.45
1:D:164[A]:GLN:CG	1:D:181:ILE:HD11	2.46	0.45
1:D:79[B]:GLU:HG3	6:D:546:HOH:O	2.17	0.44
1:B:164[B]:GLN:CD	1:B:181:ILE:HD11	2.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139[B]:THR:CG2	6:D:447:HOH:O	2.64	0.44
1:D:164[A]:GLN:CD	1:D:181:ILE:HD11	2.38	0.43
1:D:172:HIS:HE1	6:D:617:HOH:O	2.04	0.41
1:A:109[A]:THR:OG1	1:C:164[A]:GLN:NE2	2.53	0.41
1:B:63:CYS:HB2	1:B:70:TYR:CE1	2.56	0.41
1:A:265:LYS:HG2	6:A:477:HOH:O	2.19	0.41

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	299/293 (102%)	290 (97%)	9 (3%)	0	100	100
1	B	300/293 (102%)	292 (97%)	8 (3%)	0	100	100
1	C	302/293 (103%)	294 (97%)	8 (3%)	0	100	100
1	D	301/293 (103%)	292 (97%)	9 (3%)	0	100	100
All	All	1202/1172 (103%)	1168 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	242/233 (104%)	240 (99%)	2 (1%)	86	83
1	B	243/233 (104%)	241 (99%)	2 (1%)	86	83
1	C	245/233 (105%)	243 (99%)	2 (1%)	86	83
1	D	244/233 (105%)	242 (99%)	2 (1%)	86	83
All	All	974/932 (104%)	966 (99%)	8 (1%)	93	83

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65[A]	LEU
1	A	65[B]	LEU
1	B	65[A]	LEU
1	B	65[B]	LEU
1	C	65[A]	LEU
1	C	65[B]	LEU
1	D	65[A]	LEU
1	D	65[B]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	43	ASN
1	A	55	ASN
1	A	98	GLN
1	A	114	GLN
1	A	164	GLN
1	A	172	HIS
1	B	36	GLN
1	B	43	ASN
1	B	98	GLN
1	B	114	GLN
1	B	172	HIS
1	C	36	GLN
1	C	43	ASN
1	C	55	ASN
1	C	98	GLN
1	C	114	GLN
1	C	172	HIS
1	C	196	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	36	GLN
1	D	43	ASN
1	D	98	GLN
1	D	114	GLN
1	D	172	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	215	1	7,8,9	1.09	0	7,11,13	1.91	1 (14%)
1	OCS	B	215	1	7,8,9	1.15	1 (14%)	7,11,13	2.38	2 (28%)
1	OCS	C	215	1	7,8,9	1.00	0	7,11,13	1.98	1 (14%)
1	OCS	D	215	1	7,8,9	1.01	0	7,11,13	2.05	2 (28%)

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	215	1	-	0/4/7/9	0/0/0/0
1	OCS	B	215	1	-	0/4/7/9	0/0/0/0
1	OCS	C	215	1	-	0/4/7/9	0/0/0/0
1	OCS	D	215	1	-	0/4/7/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	215	OCS	OD2-SG	-2.03	1.41	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	215	OCS	OD1-SG-CB	-2.05	105.21	106.94
1	B	215	OCS	OD3-SG-CB	3.77	110.12	106.94
1	A	215	OCS	OD3-SG-CB	4.01	110.32	106.94
1	C	215	OCS	OD3-SG-CB	4.40	110.65	106.94
1	B	215	OCS	OD1-SG-CB	4.49	110.72	106.94
1	D	215	OCS	OD3-SG-CB	4.55	110.77	106.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

36 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	FUC	A	294	2	11,11,11	0.54	0	16,16,16	0.93	1 (6%)
2	GAL	A	295	2	11,11,12	0.86	0	15,15,17	0.68	0
2	GLA	A	296	2	11,11,12	0.84	0	14,15,17	0.60	0
2	FUC	A	297	2	11,11,11	0.59	0	16,16,16	0.51	0
2	GAL	A	298	2	11,11,12	0.76	0	15,15,17	1.08	1 (6%)
2	GLA	A	299	2	11,11,12	0.49	0	14,15,17	1.09	1 (7%)
3	FUC	A	300	3	11,11,11	0.64	0	16,16,16	0.85	0
3	GLA	A	301	3	11,11,12	0.90	0	15,15,17	0.98	0
3	GLA	A	302	3	11,11,12	0.73	0	14,15,17	1.07	2 (14%)
2	FUC	B	294	2	11,11,11	0.56	0	16,16,16	0.87	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	B	295	2	11,11,12	0.76	0	15,15,17	1.02	1 (6%)
2	GLA	B	296	2	11,11,12	0.78	0	14,15,17	0.99	0
2	FUC	B	297	2	11,11,11	0.55	0	16,16,16	0.44	0
2	GAL	B	298	2	11,11,12	0.83	0	15,15,17	1.05	1 (6%)
2	GLA	B	299	2	11,11,12	0.58	0	14,15,17	1.07	1 (7%)
3	FUC	B	300	3	11,11,11	0.57	0	16,16,16	0.67	0
3	GLA	B	301	3	11,11,12	0.88	0	15,15,17	0.82	0
3	GLA	B	302	3	11,11,12	0.65	0	14,15,17	0.69	0
2	FUC	C	294	2	11,11,11	0.51	0	16,16,16	0.85	1 (6%)
2	GAL	C	295	2	11,11,12	0.69	0	15,15,17	0.92	1 (6%)
2	GLA	C	296	2	11,11,12	0.70	0	14,15,17	0.68	0
2	FUC	C	297	2	11,11,11	0.47	0	16,16,16	0.51	0
2	GAL	C	298	2	11,11,12	0.74	0	15,15,17	1.16	1 (6%)
2	GLA	C	299	2	11,11,12	0.52	0	14,15,17	0.94	1 (7%)
3	FUC	C	300	3	11,11,11	0.61	0	16,16,16	0.86	0
3	GLA	C	301	3	11,11,12	1.03	1 (9%)	15,15,17	0.91	0
3	GLA	C	302	3	11,11,12	0.67	0	14,15,17	0.95	2 (14%)
2	FUC	D	294	2	11,11,11	0.58	0	16,16,16	0.80	1 (6%)
2	GAL	D	295	2	11,11,12	0.81	0	15,15,17	0.94	1 (6%)
2	GLA	D	296	2	11,11,12	0.89	0	14,15,17	1.00	2 (14%)
2	FUC	D	297	2	11,11,11	0.53	0	16,16,16	0.54	0
2	GAL	D	298	2	11,11,12	0.76	0	15,15,17	1.09	1 (6%)
2	GLA	D	299	2	11,11,12	0.51	0	14,15,17	0.94	1 (7%)
3	FUC	D	300	3	11,11,11	0.61	0	16,16,16	0.75	0
3	GLA	D	301	3	11,11,12	0.96	1 (9%)	15,15,17	0.88	0
3	GLA	D	302	3	11,11,12	0.67	0	14,15,17	0.87	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	FUC	A	294	2	-	0/0/20/20	0/1/1/1
2	GAL	A	295	2	-	0/2/18/22	0/1/1/1
2	GLA	A	296	2	-	0/2/19/22	0/1/1/1
2	FUC	A	297	2	-	0/0/20/20	0/1/1/1
2	GAL	A	298	2	-	0/2/18/22	0/1/1/1
2	GLA	A	299	2	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	A	300	3	-	0/0/20/20	0/1/1/1
3	GLA	A	301	3	-	0/2/18/22	0/1/1/1
3	GLA	A	302	3	-	0/2/19/22	0/1/1/1
2	FUC	B	294	2	-	0/0/20/20	0/1/1/1
2	GAL	B	295	2	-	0/2/18/22	0/1/1/1
2	GLA	B	296	2	-	0/2/19/22	0/1/1/1
2	FUC	B	297	2	-	0/0/20/20	0/1/1/1
2	GAL	B	298	2	-	0/2/18/22	0/1/1/1
2	GLA	B	299	2	-	0/2/19/22	0/1/1/1
3	FUC	B	300	3	-	0/0/20/20	0/1/1/1
3	GLA	B	301	3	-	0/2/18/22	0/1/1/1
3	GLA	B	302	3	-	0/2/19/22	0/1/1/1
2	FUC	C	294	2	-	0/0/20/20	0/1/1/1
2	GAL	C	295	2	-	0/2/18/22	0/1/1/1
2	GLA	C	296	2	-	0/2/19/22	0/1/1/1
2	FUC	C	297	2	-	0/0/20/20	0/1/1/1
2	GAL	C	298	2	-	0/2/18/22	0/1/1/1
2	GLA	C	299	2	-	0/2/19/22	0/1/1/1
3	FUC	C	300	3	-	0/0/20/20	0/1/1/1
3	GLA	C	301	3	-	0/2/18/22	0/1/1/1
3	GLA	C	302	3	-	0/2/19/22	0/1/1/1
2	FUC	D	294	2	-	0/0/20/20	0/1/1/1
2	GAL	D	295	2	-	0/2/18/22	0/1/1/1
2	GLA	D	296	2	-	0/2/19/22	0/1/1/1
2	FUC	D	297	2	-	0/0/20/20	0/1/1/1
2	GAL	D	298	2	-	0/2/18/22	0/1/1/1
2	GLA	D	299	2	-	0/2/19/22	0/1/1/1
3	FUC	D	300	3	-	0/0/20/20	0/1/1/1
3	GLA	D	301	3	-	0/2/18/22	0/1/1/1
3	GLA	D	302	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	GLA	O1-C1	2.03	1.44	1.39
3	C	301	GLA	O1-C1	2.22	1.44	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	298	GAL	C3-C4-C5	-3.21	106.70	109.93
2	D	298	GAL	C3-C4-C5	-3.01	106.91	109.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	298	GAL	C3-C4-C5	-2.84	107.07	109.93
2	D	295	GAL	O5-C1-C2	-2.73	108.60	110.72
2	B	298	GAL	C3-C4-C5	-2.57	107.34	109.93
2	C	295	GAL	O5-C1-C2	-2.53	108.75	110.72
2	B	295	GAL	O5-C1-C2	-2.35	108.89	110.72
2	D	296	GLA	C1-O5-C5	2.01	114.80	112.25
3	D	302	GLA	C1-O5-C5	2.05	114.85	112.25
2	D	296	GLA	C1-C2-C3	2.11	112.03	109.54
3	C	302	GLA	C1-O5-C5	2.16	114.99	112.25
3	A	302	GLA	O2-C2-C3	2.22	114.58	110.12
3	C	302	GLA	O2-C2-C3	2.25	114.65	110.12
2	D	294	FUC	O5-C1-C2	2.37	113.58	109.80
2	B	299	GLA	C1-O5-C5	2.41	115.30	112.25
2	C	294	FUC	O5-C1-C2	2.52	113.81	109.80
2	B	294	FUC	O5-C1-C2	2.77	114.21	109.80
2	A	294	FUC	O5-C1-C2	2.78	114.23	109.80
2	C	299	GLA	C1-O5-C5	2.80	115.81	112.25
2	D	299	GLA	C1-O5-C5	2.85	115.87	112.25
3	A	302	GLA	C1-O5-C5	2.89	115.91	112.25
2	A	299	GLA	C1-O5-C5	3.17	116.27	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 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	ACT	A	306	-	1,3,3	0.17	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	A	309	-	1,3,3	0.15	0	0,3,3	0.00	-
5	ACT	C	306	-	1,3,3	0.17	0	0,3,3	0.00	-
5	ACT	D	304	-	1,3,3	0.22	0	0,3,3	0.00	-

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	ACT	A	306	-	-	0/0/0/0	0/0/0/0
5	ACT	A	309	-	-	0/0/0/0	0/0/0/0
5	ACT	C	306	-	-	0/0/0/0	0/0/0/0
5	ACT	D	304	-	-	0/0/0/0	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.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	306	ACT	2	0
5	A	309	ACT	1	0
5	C	306	ACT	2	0
5	D	304	ACT	4	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	291/293 (99%)	-0.77	2 (0%) 89 87	6, 9, 18, 28	0
1	B	291/293 (99%)	-0.78	2 (0%) 89 87	6, 9, 18, 28	0
1	C	291/293 (99%)	-0.79	0 100 100	6, 9, 18, 28	0
1	D	291/293 (99%)	-0.79	2 (0%) 89 87	6, 9, 18, 27	0
All	All	1164/1172 (99%)	-0.78	6 (0%) 91 90	6, 9, 18, 28	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	GLY	2.6
1	D	205	GLY	2.6
1	B	55	ASN	2.3
1	B	205	GLY	2.2
1	D	55	ASN	2.1
1	A	55	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	OCS	D	215	9/10	0.95	0.10	-	6,8,9,11	4
1	OCS	C	215	9/10	0.97	0.09	-	7,7,11,11	4
1	OCS	B	215	9/10	0.96	0.08	-	7,8,9,11	4
1	OCS	A	215	9/10	0.96	0.09	-	5,8,9,10	4

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GLA	C	299	11/12	0.97	0.07	0.89	12,12,14,16	0
2	GAL	A	298	11/12	0.95	0.08	0.81	8,10,14,18	0
2	GAL	B	298	11/12	0.96	0.07	0.49	8,10,14,19	0
2	GLA	D	299	11/12	0.98	0.06	0.45	11,12,13,14	0
2	GAL	D	298	11/12	0.97	0.08	0.40	8,10,14,19	0
2	GAL	C	298	11/12	0.96	0.07	0.18	9,10,14,19	0
2	GAL	D	295	11/12	0.98	0.06	0.01	4,6,8,9	0
2	GLA	A	296	11/12	0.98	0.06	-0.02	3,6,6,7	0
2	GLA	A	299	11/12	0.97	0.06	-0.07	11,13,14,16	0
3	GLA	A	301	11/12	0.98	0.06	-0.07	6,7,10,12	0
2	GLA	C	296	11/12	0.99	0.06	-0.08	4,5,6,7	0
2	GAL	C	295	11/12	0.99	0.06	-0.10	4,7,9,11	0
2	GAL	A	295	11/12	0.98	0.06	-0.26	4,6,7,10	0
3	GLA	B	301	11/12	0.98	0.06	-0.28	7,7,10,12	0
2	GAL	B	295	11/12	0.99	0.06	-0.29	3,7,8,9	0
3	GLA	C	302	11/12	0.98	0.06	-0.45	8,10,11,14	0
3	GLA	A	302	11/12	0.98	0.06	-0.47	7,8,11,12	0
2	GLA	D	296	11/12	0.99	0.06	-0.56	4,6,7,7	0
2	GLA	B	296	11/12	0.99	0.05	-0.61	4,5,7,7	0
3	GLA	D	301	11/12	0.98	0.06	-0.82	7,7,10,11	0
3	GLA	D	302	11/12	0.99	0.05	-1.04	8,9,11,12	0
3	GLA	B	302	11/12	0.99	0.04	-1.13	8,9,11,12	0
2	GLA	B	299	11/12	0.99	0.05	-1.14	12,12,13,14	0
3	GLA	C	301	11/12	0.99	0.05	-1.30	6,7,9,10	0
3	FUC	D	300	11/11	0.97	0.07	-	10,17,20,22	0
3	FUC	C	300	11/11	0.97	0.06	-	10,17,21,23	0
2	FUC	D	294	11/11	0.98	0.06	-	9,11,13,13	0
2	FUC	B	294	11/11	0.97	0.07	-	8,11,13,13	0
3	FUC	A	300	11/11	0.97	0.07	-	11,17,21,22	0
2	FUC	A	294	11/11	0.97	0.07	-	8,11,12,13	0
2	FUC	A	297	11/11	0.97	0.07	-	15,18,20,22	0
2	FUC	D	297	11/11	0.96	0.08	-	15,19,21,22	0
2	FUC	C	294	11/11	0.97	0.08	-	9,12,13,13	0
2	FUC	C	297	11/11	0.96	0.08	-	14,19,21,22	0
3	FUC	B	300	11/11	0.97	0.06	-	11,18,21,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FUC	B	297	11/11	0.97	0.07	-	13,18,21,21	0

6.4 Ligands [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	ACT	A	309	4/4	0.86	0.17	10.24	23,23,24,25	0
5	ACT	A	306	4/4	0.85	0.17	8.40	22,22,22,23	0
5	ACT	C	306	4/4	0.90	0.16	7.64	21,21,22,23	0
5	ACT	D	304	4/4	0.94	0.15	5.91	15,16,16,16	1
4	CA	B	303	1/1	1.00	0.07	0.58	8,8,8,8	0
4	CA	D	303	1/1	0.99	0.07	0.32	8,8,8,8	0
4	CA	D	306	1/1	0.87	0.06	-0.36	65,65,65,65	0
4	CA	C	308	1/1	0.91	0.05	-0.53	58,58,58,58	0
4	CA	A	303	1/1	0.99	0.06	-0.58	8,8,8,8	0
4	CA	C	304	1/1	1.00	0.05	-0.81	9,9,9,9	0
4	CA	B	306	1/1	0.90	0.05	-0.86	57,57,57,57	0
4	CA	D	305	1/1	0.93	0.06	-0.97	55,55,55,55	0
4	CA	A	308	1/1	0.96	0.04	-1.16	58,58,58,58	0
4	CA	C	307	1/1	0.97	0.05	-1.34	55,55,55,55	0
4	CA	B	305	1/1	0.97	0.05	-1.62	55,55,55,55	0
4	CA	A	307	1/1	0.96	0.04	-1.63	52,52,52,52	0
4	CA	C	305	1/1	1.00	0.04	-	11,11,11,11	0
4	CA	C	303	1/1	1.00	0.04	-	11,11,11,11	0
4	CA	A	305	1/1	1.00	0.05	-	10,10,10,10	0
4	CA	A	304	1/1	1.00	0.04	-	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.