



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:26 PM GMT

PDB ID : 4OWL  
Title : Crystal Structure of the Vibrio vulnificus Hemolysin/Cytolysin Beta-Trefoil Lectin with N-Acetyl-D-Lactosamine Bound  
Authors : Kaus, K.; Olson, R.  
Deposited on : 2014-02-02  
Resolution : 2.10 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:

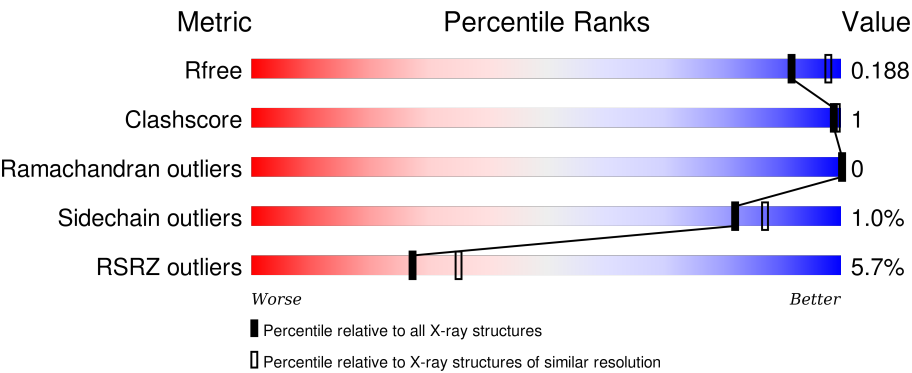
MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.10 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 <sub>free</sub>	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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.

Mol	Chain	Length	Quality of chain
1	A	138	<div><div>9%</div><div>93%</div><div>• •</div></div>
1	B	138	<div><div>10%</div><div>93%</div><div>• 5%</div></div>
1	C	138	<div><div>4%</div><div>92%</div><div>• 5%</div></div>
1	D	138	<div><div>%</div><div>96%</div><div>• • •</div></div>
1	E	138	<div><div>90%</div><div>6%</div><div>•</div></div>

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Mol	Chain	Length	Quality of chain
1	F	138	 % 91% 5% 13%
1	G	138	 13% 94% 5%

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
2	GOL	A	501	-	-	-	X
2	GOL	C	503	-	-	-	X
2	GOL	D	503	-	-	-	X
2	GOL	E	503	-	-	-	X
2	GOL	F	503	-	-	-	X
4	NAG	F	502	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14288 atoms, of which 6571 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 Cytolysin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	132	Total	C	H	N	O	S	0	0	0
			1811	599	844	175	189	4			
1	B	131	Total	C	H	N	O	S	0	0	0
			1854	603	877	178	191	5			
1	C	131	Total	C	H	N	O	S	0	0	0
			1913	613	919	183	193	5			
1	D	137	Total	C	H	N	O	S	0	0	0
			2050	657	983	196	209	5			
1	E	132	Total	C	H	N	O	S	0	0	0
			2009	636	974	191	203	5			
1	F	131	Total	C	H	N	O	S	0	0	0
			1938	616	934	186	197	5			
1	G	131	Total	C	H	N	O	S	0	0	0
			1837	599	864	179	190	5			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	GLY	-	expression tag	UNP P19247
A	335	SER	-	expression tag	UNP P19247
A	336	ALA	-	expression tag	UNP P19247
A	337	MET	-	expression tag	UNP P19247
B	334	GLY	-	expression tag	UNP P19247
B	335	SER	-	expression tag	UNP P19247
B	336	ALA	-	expression tag	UNP P19247
B	337	MET	-	expression tag	UNP P19247
C	334	GLY	-	expression tag	UNP P19247
C	335	SER	-	expression tag	UNP P19247
C	336	ALA	-	expression tag	UNP P19247
C	337	MET	-	expression tag	UNP P19247
D	334	GLY	-	expression tag	UNP P19247
D	335	SER	-	expression tag	UNP P19247
D	336	ALA	-	expression tag	UNP P19247

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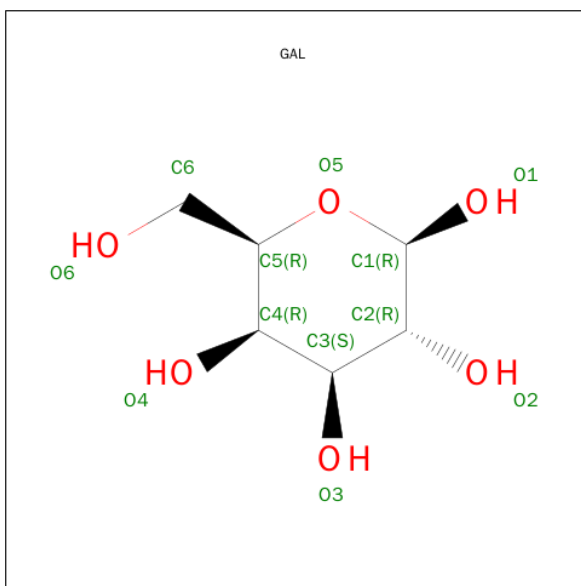
Chain	Residue	Modelled	Actual	Comment	Reference
D	337	MET	-	expression tag	UNP P19247
E	334	GLY	-	expression tag	UNP P19247
E	335	SER	-	expression tag	UNP P19247
E	336	ALA	-	expression tag	UNP P19247
E	337	MET	-	expression tag	UNP P19247
F	334	GLY	-	expression tag	UNP P19247
F	335	SER	-	expression tag	UNP P19247
F	336	ALA	-	expression tag	UNP P19247
F	337	MET	-	expression tag	UNP P19247
G	334	GLY	-	expression tag	UNP P19247
G	335	SER	-	expression tag	UNP P19247
G	336	ALA	-	expression tag	UNP P19247
G	337	MET	-	expression tag	UNP P19247

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		
2	E	1	Total	C	H	O	0	0
			14	3	8	3		
2	F	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is BETA-D-GALACTOSE (three-letter code: GAL) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			22	6	11	5		
3	C	1	Total	C	H	O	0	0
			22	6	11	5		
3	D	1	Total	C	H	O	0	0
			22	6	11	5		
3	E	1	Total	C	H	O	0	0
			22	6	11	5		
3	F	1	Total	C	H	O	0	0
			22	6	11	5		
3	G	1	Total	C	H	O	0	0
			22	6	11	5		

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	B	1	Total 29	C 8	H 14	N 1	O 6	0	0
4	C	1	Total 29	C 8	H 14	N 1	O 6	0	0
4	D	1	Total 29	C 8	H 14	N 1	O 6	0	0
4	E	1	Total 29	C 8	H 14	N 1	O 6	0	0
4	F	1	Total 29	C 8	H 14	N 1	O 6	0	0

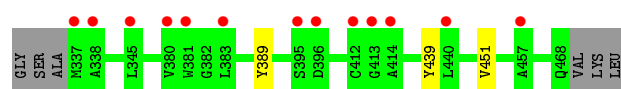
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	16	Total	O	0	0
			16	16		
5	C	62	Total	O	0	0
			62	62		
5	D	142	Total	O	0	0
			142	142		
5	E	157	Total	O	0	0
			157	157		
5	F	117	Total	O	0	0
			117	117		
5	G	24	Total	O	0	0
			24	24		

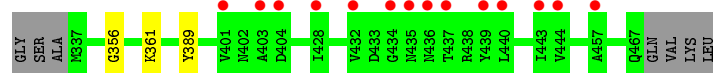
### 3 Residue-property plots [i](#)

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.

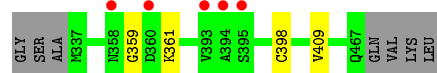
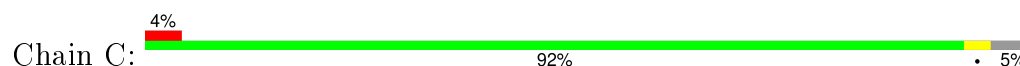
- Molecule 1: Cytolysin



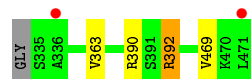
- Molecule 1: Cytolysin



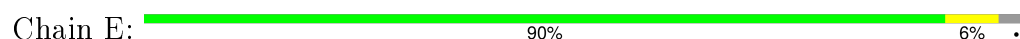
- Molecule 1: Cytolysin



- Molecule 1: Cytolysin



- Molecule 1: Cytolysin



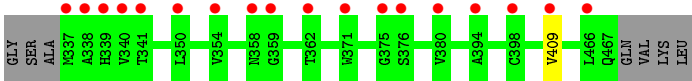
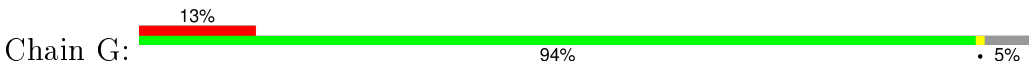
- Molecule 1: Cytolysin







● Molecule 1: Cytolysin



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	326.90Å 79.84Å 55.61Å 90.00° 95.71° 90.00°	Depositor
Resolution (Å)	40.16 – 2.10 48.02 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.16-2.10) 99.8 (48.02-2.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.94 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.162 , 0.188 0.161 , 0.188	Depositor DCC
$R_{free}$ test set	4155 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.2	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 58.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 83123 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14288	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, GAL, 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	0.37	0/985	0.52	0/1345
1	B	0.39	0/995	0.53	0/1360
1	C	0.55	0/1012	0.62	0/1378
1	D	0.88	0/1087	0.81	1/1478 (0.1%)
1	E	0.88	2/1055 (0.2%)	0.83	2/1435 (0.1%)
1	F	0.74	0/1022	0.74	1/1390 (0.1%)
1	G	0.40	0/991	0.54	0/1352
All	All	0.65	2/7147 (0.0%)	0.67	4/9738 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	387	GLU	CG-CD	5.83	1.60	1.51
1	E	456	GLU	CG-CD	5.33	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	398	CYS	CA-CB-SG	-7.86	99.86	114.00
1	D	390	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	E	397	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	F	388	ARG	NE-CZ-NH1	5.55	123.08	120.30

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	967	844	864	1	0
1	B	977	877	886	1	0
1	C	994	919	927	3	0
1	D	1067	983	1003	1	0
1	E	1035	974	975	3	0
1	F	1004	934	935	2	0
1	G	973	864	877	0	0
2	A	6	8	8	0	0
2	C	6	8	8	0	0
2	D	6	8	8	0	0
2	E	6	8	8	0	0
2	F	6	8	8	0	0
3	B	11	11	10	0	0
3	C	11	11	10	0	0
3	D	11	11	10	0	0
3	E	11	11	10	0	0
3	F	11	11	10	0	0
3	G	11	11	10	0	0
4	B	15	14	14	0	0
4	C	15	14	14	1	0
4	D	15	14	14	0	0
4	E	15	14	14	1	0
4	F	15	14	14	0	0
5	A	11	0	0	0	0
5	B	16	0	0	0	0
5	C	62	0	0	1	0
5	D	142	0	0	0	0
5	E	157	0	0	1	1
5	F	117	0	0	1	0
5	G	24	0	0	0	0
All	All	7717	6571	6637	11	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 1.

All (11) 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:392:ARG:HH11	1:D:469:VAL:HG11	1.62	0.63
1:C:361:LYS:O	5:C:653:HOH:O	2.19	0.51
1:F:356:GLY:O	5:F:703:HOH:O	2.19	0.50
1:C:359:GLY:HA3	4:C:502:NAG:H83	1.94	0.50
1:E:359:GLY:HA3	4:E:502:NAG:H83	1.96	0.47
1:A:439:TYR:HB3	1:A:451:VAL:HB	1.97	0.47
1:E:463:LYS:NZ	5:E:692:HOH:O	2.50	0.45
1:B:356:GLY:HA3	1:B:361:LYS:HA	2.00	0.44
1:F:439:TYR:HB3	1:F:451:VAL:HB	2.01	0.43
1:C:398:CYS:O	1:C:409:VAL:HA	2.19	0.41
1:E:439:TYR:HB3	1:E:451:VAL:HB	2.03	0.41

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)
5:E:619:HOH:O	5:E:623:HOH:O[4_758]	2.09	0.11

## 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	130/138 (94%)	124 (95%)	6 (5%)	0	100	100
1	B	129/138 (94%)	121 (94%)	8 (6%)	0	100	100
1	C	129/138 (94%)	125 (97%)	4 (3%)	0	100	100
1	D	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
1	E	130/138 (94%)	126 (97%)	4 (3%)	0	100	100
1	F	129/138 (94%)	126 (98%)	3 (2%)	0	100	100
1	G	129/138 (94%)	121 (94%)	8 (6%)	0	100	100
All	All	911/966 (94%)	874 (96%)	37 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	92/116 (79%)	91 (99%)	1 (1%)	80	85
1	B	97/116 (84%)	96 (99%)	1 (1%)	82	87
1	C	102/116 (88%)	102 (100%)	0	100	100
1	D	112/116 (97%)	110 (98%)	2 (2%)	66	72
1	E	110/116 (95%)	110 (100%)	0	100	100
1	F	104/116 (90%)	102 (98%)	2 (2%)	65	70
1	G	95/116 (82%)	94 (99%)	1 (1%)	80	85
All	All	712/812 (88%)	705 (99%)	7 (1%)	82	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	389	TYR
1	B	389	TYR
1	D	363	VAL
1	D	392	ARG
1	F	389	TYR
1	F	395	SER
1	G	409	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GOL	A	501	-	5,5,5	0.33	0	5,5,5	0.31	0
3	GAL	B	501	4	11,11,12	0.71	0	14,15,17	1.07	0
4	NAG	B	502	3	15,15,15	0.50	0	17,21,21	0.40	0
3	GAL	C	501	4	11,11,12	0.80	0	14,15,17	0.84	0
4	NAG	C	502	3	15,15,15	0.41	0	17,21,21	0.38	0
2	GOL	C	503	-	5,5,5	0.34	0	5,5,5	0.28	0
3	GAL	D	501	4	11,11,12	1.26	0	14,15,17	1.20	2 (14%)
4	NAG	D	502	3	15,15,15	0.73	1 (6%)	17,21,21	0.59	0
2	GOL	D	503	-	5,5,5	0.44	0	5,5,5	0.49	0
3	GAL	E	501	4	11,11,12	1.32	2 (18%)	14,15,17	1.23	1 (7%)
4	NAG	E	502	3	15,15,15	0.30	0	17,21,21	0.58	0
2	GOL	E	503	-	5,5,5	0.35	0	5,5,5	0.31	0
3	GAL	F	501	4	11,11,12	2.01	2 (18%)	14,15,17	0.93	0
4	NAG	F	502	3	15,15,15	0.56	0	17,21,21	0.41	0
2	GOL	F	503	-	5,5,5	0.32	0	5,5,5	0.33	0
3	GAL	G	501	-	11,11,12	0.95	0	14,15,17	1.24	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	GOL	A	501	-	-	0/4/4/4	0/0/0/0
3	GAL	B	501	4	-	0/2/19/22	0/1/1/1
4	NAG	B	502	3	-	0/6/26/26	0/1/1/1
3	GAL	C	501	4	-	0/2/19/22	0/1/1/1
4	NAG	C	502	3	-	0/6/26/26	0/1/1/1
2	GOL	C	503	-	-	0/4/4/4	0/0/0/0
3	GAL	D	501	4	-	0/2/19/22	0/1/1/1
4	NAG	D	502	3	-	0/6/26/26	0/1/1/1
2	GOL	D	503	-	-	0/4/4/4	0/0/0/0
3	GAL	E	501	4	-	0/2/19/22	0/1/1/1
4	NAG	E	502	3	-	0/6/26/26	0/1/1/1
2	GOL	E	503	-	-	0/4/4/4	0/0/0/0
3	GAL	F	501	4	-	0/2/19/22	0/1/1/1
4	NAG	F	502	3	-	0/6/26/26	0/1/1/1
2	GOL	F	503	-	-	0/4/4/4	0/0/0/0
3	GAL	G	501	-	-	0/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	501	GAL	C2-C3	-5.20	1.45	1.52
4	D	502	NAG	C1-C2	-2.16	1.50	1.53
3	E	501	GAL	C2-C3	-2.13	1.49	1.52
3	E	501	GAL	C4-C3	2.15	1.58	1.52
3	F	501	GAL	O3-C3	2.45	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	GAL	O2-C2-C3	-2.65	104.79	110.12
3	D	501	GAL	O5-C5-C6	-2.05	102.90	107.35
3	E	501	GAL	C1-C2-C3	2.74	112.78	109.54
3	G	501	GAL	C1-O5-C5	2.90	115.93	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	NAG	1	0
4	E	502	NAG	1	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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	132/138 (95%)	0.77	13 (9%) 10 13	57, 74, 101, 115	0
1	B	131/138 (94%)	0.61	14 (10%) 8 11	54, 72, 93, 113	0
1	C	131/138 (94%)	0.33	5 (3%) 44 53	28, 54, 84, 101	0
1	D	137/138 (99%)	0.36	2 (1%) 76 81	19, 27, 58, 85	0
1	E	132/138 (95%)	0.44	0 100 100	17, 26, 44, 67	0
1	F	131/138 (94%)	0.02	1 (0%) 87 90	21, 35, 55, 66	0
1	G	131/138 (94%)	0.80	18 (13%) 4 5	42, 72, 95, 122	0
All	All	925/966 (95%)	0.47	53 (5%) 27 35	17, 54, 91, 122	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	337	MET	4.9
1	B	437	THR	4.8
1	G	466	LEU	4.8
1	A	413	GLY	4.7
1	B	434	GLY	4.4
1	G	337	MET	4.4
1	A	412	CYS	4.3
1	G	362	THR	4.0
1	G	371	TRP	3.9
1	G	339	HIS	3.9
1	B	403	ALA	3.8
1	B	440	LEU	3.7
1	G	340	VAL	3.7
1	G	338	ALA	3.6
1	G	376	SER	3.5
1	C	394	ALA	3.5
1	B	439	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	354	VAL	3.2
1	G	380	VAL	3.1
1	C	358	ASN	3.1
1	A	338	ALA	3.1
1	A	396	ASP	3.1
1	G	359	GLY	2.9
1	C	360	ASP	2.9
1	G	341	THR	2.9
1	G	350	LEU	2.8
1	G	375	GLY	2.8
1	F	337	MET	2.7
1	B	457	ALA	2.6
1	C	393	VAL	2.6
1	A	414	ALA	2.6
1	A	345	LEU	2.5
1	A	383	LEU	2.5
1	B	436	ASN	2.5
1	D	471	LEU	2.4
1	B	443	ILE	2.3
1	B	435	ASN	2.3
1	G	358	ASN	2.3
1	B	401	VAL	2.3
1	B	428	ILE	2.3
1	A	440	LEU	2.3
1	A	395	SER	2.2
1	D	336	ALA	2.2
1	A	381	TRP	2.1
1	G	409	VAL	2.1
1	A	380	VAL	2.1
1	G	398	CYS	2.1
1	G	394	ALA	2.1
1	A	457	ALA	2.1
1	C	395	SER	2.1
1	B	432	VAL	2.1
1	B	444	VAL	2.1
1	B	404	ASP	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	GOL	F	503	6/6	0.81	0.29	16.63	73,88,90,91	0
2	GOL	C	503	6/6	0.82	0.40	14.31	79,95,99,102	0
2	GOL	D	503	6/6	0.76	0.33	9.78	53,64,69,73	0
2	GOL	E	503	6/6	0.74	0.25	6.70	62,74,77,77	0
4	NAG	F	502	15/15	0.94	0.18	5.46	55,72,88,89	0
2	GOL	A	501	6/6	0.85	0.19	5.07	78,93,97,100	0
4	NAG	E	502	15/15	0.84	0.19	1.69	50,72,88,88	0
4	NAG	D	502	15/15	0.91	0.14	0.62	42,55,66,72	0
3	GAL	G	501	11/12	0.89	0.23	0.25	92,103,120,123	0
4	NAG	C	502	15/15	0.81	0.20	0.08	85,106,130,130	0
3	GAL	F	501	11/12	0.96	0.11	-0.30	38,46,53,56	0
3	GAL	C	501	11/12	0.88	0.12	-0.52	60,71,82,86	0
3	GAL	B	501	11/12	0.91	0.10	-1.19	79,88,102,106	0
3	GAL	D	501	11/12	0.97	0.13	-1.28	26,33,39,43	0
3	GAL	E	501	11/12	0.99	0.12	-2.34	25,32,38,44	0
4	NAG	B	502	15/15	0.76	0.28	-	97,112,137,137	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.