wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 08:02 PM EDT

PDB ID	:	3V4V
Title	:	crystal structure of a4b7 headpiece complexed with Fab ACT-1 and RO0505376
Authors	:	Yu, Y.; Zhu, J.; Springer, T.A.
Deposited on	:	2011-12-15
Resolution	:	3.10 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

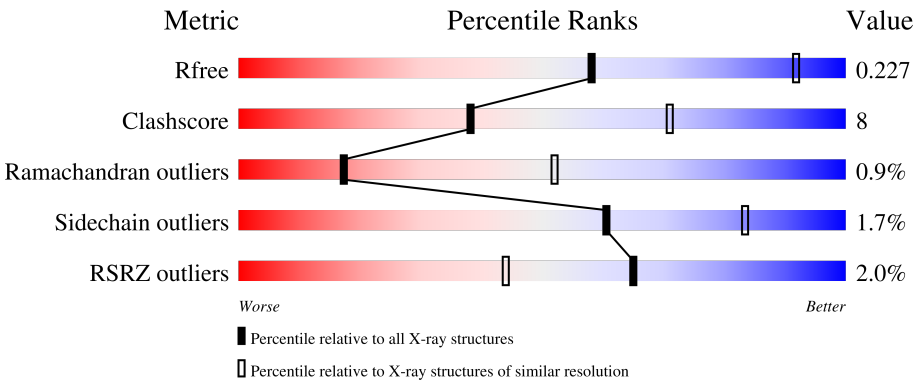
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	597	% 74% 23% • •
1	C	597	% 72% 24% • •
2	B	503	% 61% 13% • 25%
2	D	503	% 61% 13% • 25%
3	H	219	6% 79% 16% • •

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Mol	Chain	Length	Quality of chain
3	M	219	82% 14%
4	L	217	8% 87% 13%
4	N	217	86% 14%
5	E	4	50% 25% 25%
5	F	4	25% 75%

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	BMA	F	3	-	-	-	X
5	MAN	F	4	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 21791 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 Integrin alpha-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	582	4499	2837	776	864	22	10	0	0
1	C	580	4489	2831	775	861	22	10	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	558	ALA	ARG	engineered mutation	UNP P13612
A	588	THR	-	expression tag	UNP P13612
A	589	GLY	-	expression tag	UNP P13612
A	590	GLY	-	expression tag	UNP P13612
A	591	LEU	-	expression tag	UNP P13612
A	592	GLU	-	expression tag	UNP P13612
A	593	ASN	-	expression tag	UNP P13612
A	594	LEU	-	expression tag	UNP P13612
A	595	TYR	-	expression tag	UNP P13612
A	596	PHE	-	expression tag	UNP P13612
A	597	GLN	-	expression tag	UNP P13612
C	558	ALA	ARG	engineered mutation	UNP P13612
C	588	THR	-	expression tag	UNP P13612
C	589	GLY	-	expression tag	UNP P13612
C	590	GLY	-	expression tag	UNP P13612
C	591	LEU	-	expression tag	UNP P13612
C	592	GLU	-	expression tag	UNP P13612
C	593	ASN	-	expression tag	UNP P13612
C	594	LEU	-	expression tag	UNP P13612
C	595	TYR	-	expression tag	UNP P13612
C	596	PHE	-	expression tag	UNP P13612
C	597	GLN	-	expression tag	UNP P13612

- Molecule 2 is a protein called Integrin beta-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	375	2918	1826	521	559	12	0	1	0
2	D	375	2919	1826	521	560	12	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	494	SER	-	expression tag	UNP P26010
B	495	ARG	-	expression tag	UNP P26010
B	496	GLY	-	expression tag	UNP P26010
B	497	LEU	-	expression tag	UNP P26010
B	498	GLU	-	expression tag	UNP P26010
B	499	ASN	-	expression tag	UNP P26010
B	500	LEU	-	expression tag	UNP P26010
B	501	TYR	-	expression tag	UNP P26010
B	502	PHE	-	expression tag	UNP P26010
B	503	GLN	-	expression tag	UNP P26010
D	494	SER	-	expression tag	UNP P26010
D	495	ARG	-	expression tag	UNP P26010
D	496	GLY	-	expression tag	UNP P26010
D	497	LEU	-	expression tag	UNP P26010
D	498	GLU	-	expression tag	UNP P26010
D	499	ASN	-	expression tag	UNP P26010
D	500	LEU	-	expression tag	UNP P26010
D	501	TYR	-	expression tag	UNP P26010
D	502	PHE	-	expression tag	UNP P26010
D	503	GLN	-	expression tag	UNP P26010

- Molecule 3 is a protein called MONOCLONAL ANTIBODY Act-1 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	211	1607	1021	258	321	7	0	0	0
3	M	213	1622	1030	261	324	7	8	0	0

- Molecule 4 is a protein called MONOCLONAL ANTIBODY Act-1 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	217	1681	1054	282	339	6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	N	217	1681	1054	282	339	6	0	0	0

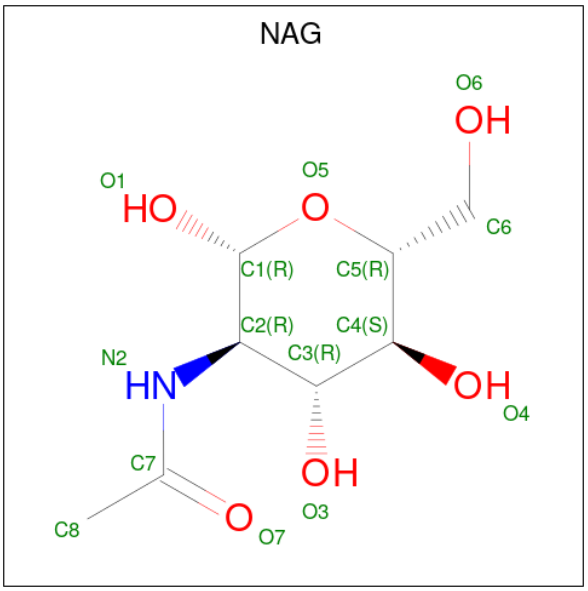
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	4	50	28	2	20	0	0	0
5	F	4	50	28	2	20	0	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

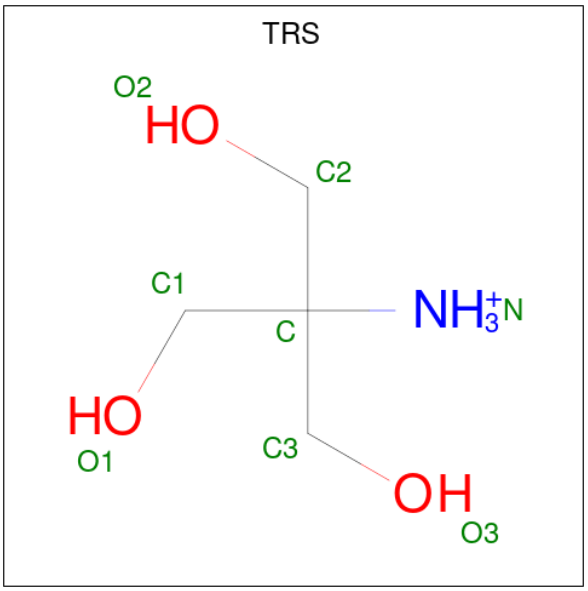
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	A	3	3	3	0	0
6	B	2	2	2	0	0
6	C	3	3	3	0	0
6	D	2	2	2	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	14	8	1	5	0	0
7	A	1	14	8	1	5	0	0
7	A	1	14	8	1	5	0	0
7	A	1	14	8	1	5	0	0
7	B	1	14	8	1	5	0	0
7	B	1	14	8	1	5	0	0
7	C	1	14	8	1	5	0	0
7	C	1	14	8	1	5	0	0
7	C	1	14	8	1	5	0	0
7	C	1	14	8	1	5	0	0
7	D	1	14	8	1	5	0	0

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

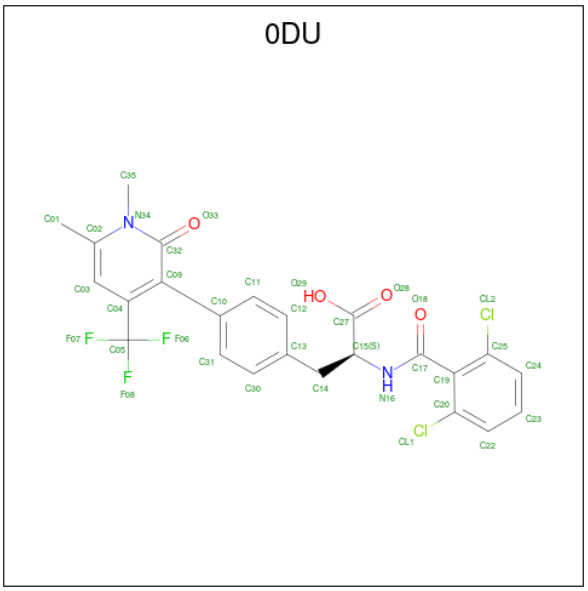


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	8	4	1	3	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
9	B	1	1	1	0	0
9	D	1	1	1	0	0

- Molecule 10 is N-(2,6-dichlorobenzoyl)-4-[1,6-dimethyl-2-oxo-4-(trifluoromethyl)-1,2-dihydropyridin-3-yl]-L-phenylalanine (three-letter code: 0DU) (formula: $C_{24}H_{19}Cl_2F_3N_2O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	F	N	O		
10	B	1	35	24	2	3	2	4	0	0
10	D	1	35	24	2	3	2	4	0	0

- Molecule 11 is water.

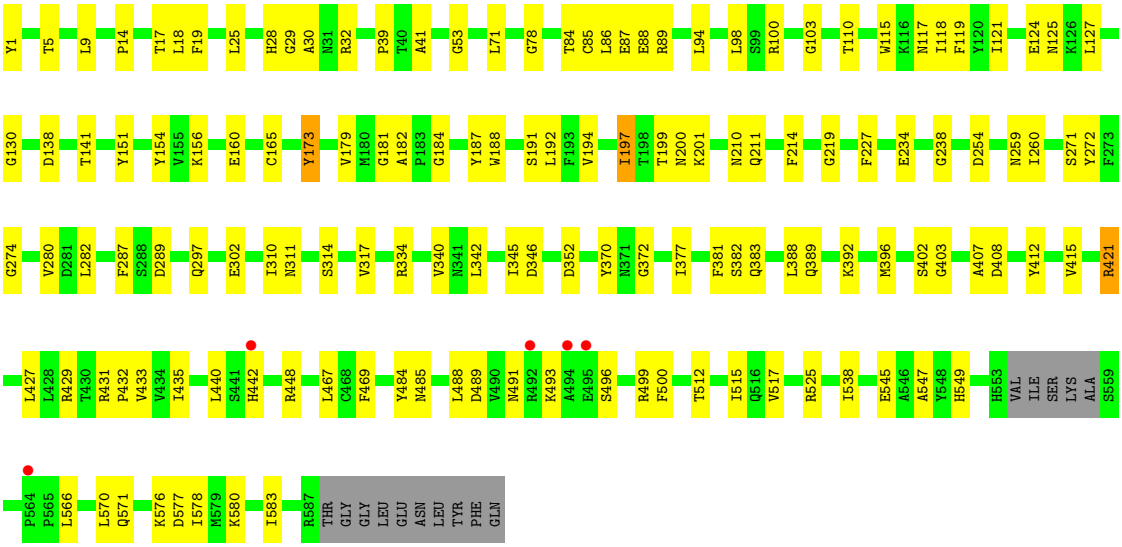
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	10	10	10	0	0
11	B	4	4	4	0	0
11	H	1	1	1	0	0
11	C	11	11	11	0	0
11	D	5	5	5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

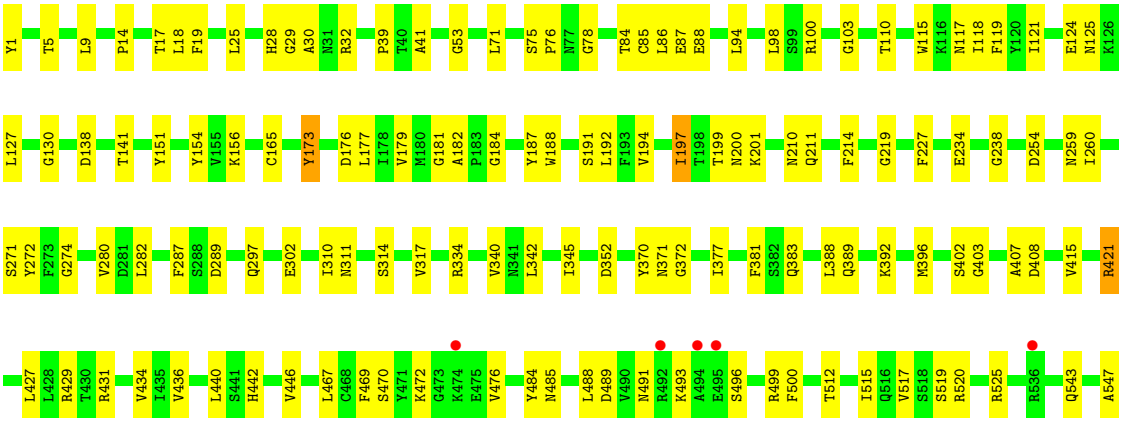
• Molecule 1: Integrin alpha-4

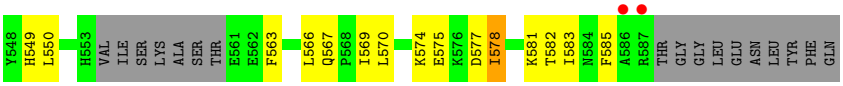
Chain A:



• Molecule 1: Integrin alpha-4

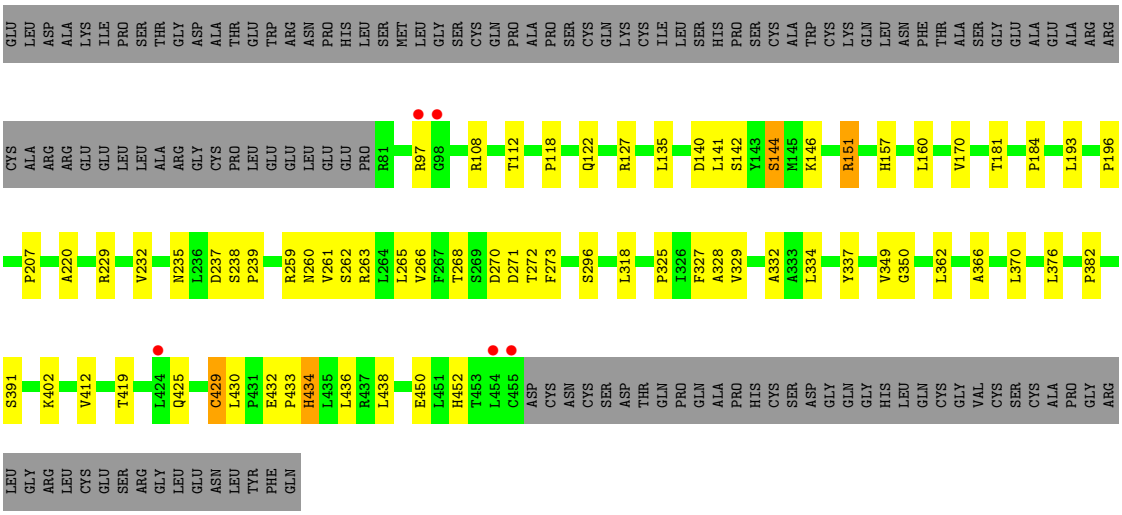
Chain C:





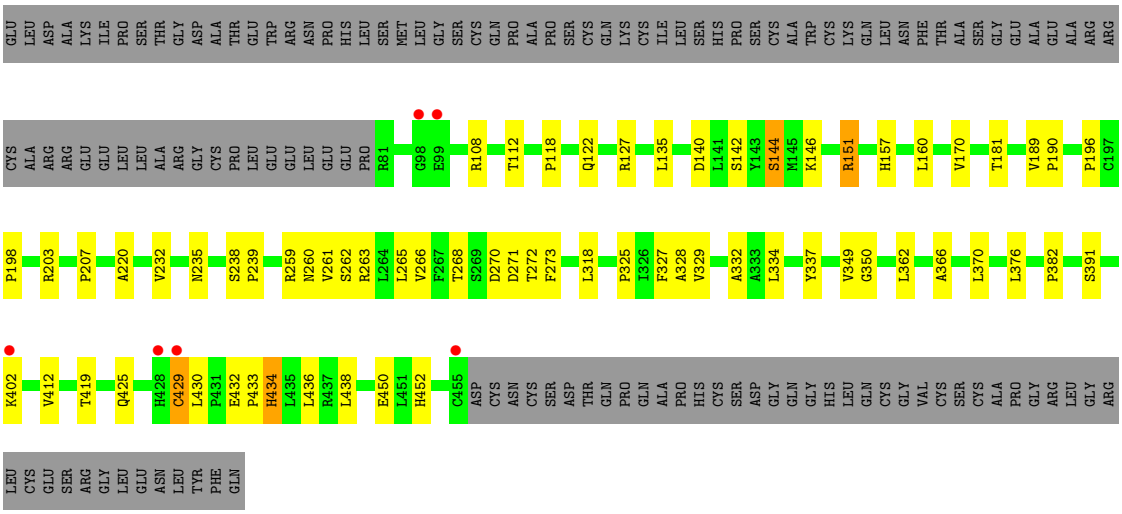
• Molecule 2: Integrin beta-7

Chain B:



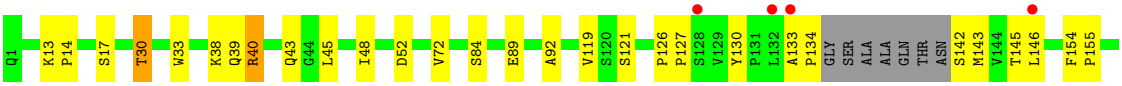
• Molecule 2: Integrin beta-7

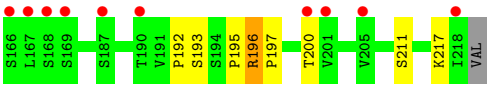
Chain D:



• Molecule 3: MONOCLONAL ANTIBODY Act-1 HEAVY CHAIN

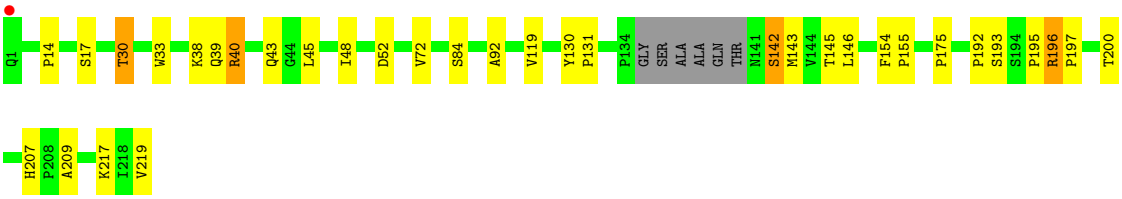
Chain H:





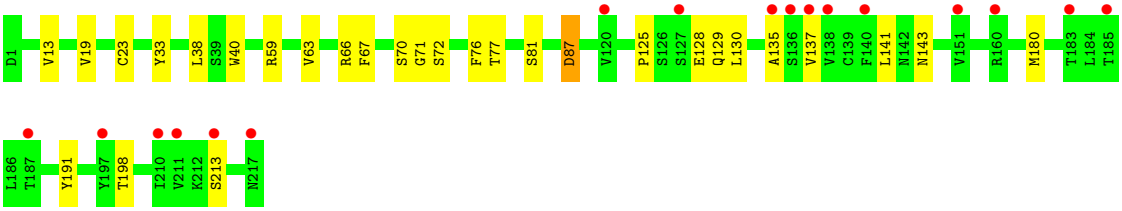
• Molecule 3: MONOCLONAL ANTIBODY Act-1 HEAVY CHAIN

Chain M:



• Molecule 4: MONOCLONAL ANTIBODY Act-1 LIGHT CHAIN

Chain L:



• Molecule 4: MONOCLONAL ANTIBODY Act-1 LIGHT CHAIN

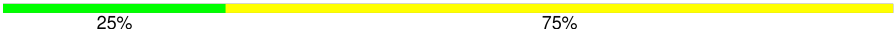
Chain N:

• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	127.58Å 123.53Å 154.16Å 90.00° 112.63° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10 56.66 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-3.10) 98.5 (56.66-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 3.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.197 , 0.231 0.193 , 0.227	Depositor DCC
R_{free} test set	1034 reflections (1.31%)	wwPDB-VP
Wilson B-factor (Å^2)	76.3	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 63.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21791	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: CA, NAG, BMA, MAN, 0DU, MG, TRS

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	0.40	4/4599 (0.1%)	0.47	1/6228 (0.0%)
1	C	0.40	4/4589 (0.1%)	0.47	1/6214 (0.0%)
2	B	0.25	0/2980	0.44	0/4046
2	D	0.25	0/2981	0.44	0/4047
3	H	0.24	0/1652	0.57	3/2259 (0.1%)
3	M	0.23	0/1667	0.57	3/2280 (0.1%)
4	L	0.24	0/1722	0.41	0/2340
4	N	0.24	0/1722	0.41	0/2340
All	All	0.32	8/21912 (0.0%)	0.47	8/29754 (0.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	19	PHE	CE2-CZ	-11.35	1.15	1.37
1	A	19	PHE	CE1-CZ	-11.23	1.16	1.37
1	C	19	PHE	CE1-CZ	-11.21	1.16	1.37
1	A	19	PHE	CE2-CZ	-11.12	1.16	1.37
1	C	19	PHE	CG-CD2	-10.19	1.23	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	40	ARG	NE-CZ-NH2	-12.14	114.23	120.30
3	M	40	ARG	NE-CZ-NH1	-12.11	114.25	120.30
3	M	40	ARG	NE-CZ-NH2	12.09	126.34	120.30
3	H	40	ARG	NE-CZ-NH1	11.46	126.03	120.30
3	M	40	ARG	CD-NE-CZ	6.12	132.17	123.60

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	4499	0	4362	82	0
1	C	4489	0	4353	86	0
2	B	2918	0	2849	44	0
2	D	2919	0	2850	38	0
3	H	1607	0	1552	23	0
3	M	1622	0	1567	22	0
4	L	1681	0	1616	20	0
4	N	1681	0	1616	21	0
5	E	50	0	43	1	0
5	F	50	0	43	1	0
6	A	3	0	0	0	0
6	B	2	0	0	0	0
6	C	3	0	0	0	0
6	D	2	0	0	0	0
7	A	56	0	52	1	0
7	B	28	0	26	1	0
7	C	56	0	52	0	0
7	D	14	0	13	0	0
8	A	8	0	12	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	B	35	0	18	2	0
10	D	35	0	18	2	0
11	A	10	0	0	1	0
11	B	4	0	0	0	0
11	C	11	0	0	3	0
11	D	5	0	0	0	0
11	H	1	0	0	0	0
All	All	21791	0	21042	326	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 8.

The worst 5 of 326 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)
3:M:196:ARG:HD2	3:M:197:PRO:HA	1.54	0.89
3:H:196:ARG:HD2	3:H:197:PRO:HA	1.55	0.85
1:C:442:HIS:HE1	1:C:583:ILE:HB	1.45	0.81
1:C:372:GLY:HA2	1:C:377:ILE:HG22	1.66	0.77
1:A:372:GLY:HA2	1:A:377:ILE:HG22	1.64	0.77

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	578/597 (97%)	523 (90%)	51 (9%)	4 (1%)	22	57
1	C	576/597 (96%)	521 (90%)	49 (8%)	6 (1%)	15	49
2	B	374/503 (74%)	337 (90%)	33 (9%)	4 (1%)	14	46
2	D	374/503 (74%)	333 (89%)	37 (10%)	4 (1%)	14	46
3	H	207/219 (94%)	185 (89%)	21 (10%)	1 (0%)	29	64
3	M	209/219 (95%)	189 (90%)	19 (9%)	1 (0%)	29	64
4	L	215/217 (99%)	197 (92%)	16 (7%)	2 (1%)	17	52
4	N	215/217 (99%)	196 (91%)	17 (8%)	2 (1%)	17	52
All	All	2748/3072 (90%)	2481 (90%)	243 (9%)	24 (1%)	17	52

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	C	200	ASN
1	C	577	ASP
1	C	578	ILE
3	M	142	SER

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	487/500 (97%)	481 (99%)	6 (1%)	71	88
1	C	486/500 (97%)	478 (98%)	8 (2%)	62	84
2	B	324/431 (75%)	316 (98%)	8 (2%)	47	75
2	D	324/431 (75%)	316 (98%)	8 (2%)	47	75
3	H	183/188 (97%)	179 (98%)	4 (2%)	52	78
3	M	185/188 (98%)	181 (98%)	4 (2%)	52	78
4	L	194/194 (100%)	193 (100%)	1 (0%)	88	94
4	N	194/194 (100%)	193 (100%)	1 (0%)	88	94
All	All	2377/2626 (90%)	2337 (98%)	40 (2%)	60	83

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	151	ARG
3	M	30	THR
2	D	170	VAL
2	D	265	LEU
3	M	145	THR

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

Mol	Chain	Res	Type
1	C	210	ASN
1	C	389	GLN
1	C	244	GLN
1	C	404	GLN
1	A	347	ASN

5.3.3 RNA (i)

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)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	E	1	1,5	14,14,15	0.57	0	17,19,21	1.02	1 (5%)
5	NAG	E	2	5	14,14,15	0.57	0	17,19,21	0.72	0
5	BMA	E	3	5	11,11,12	0.53	0	15,15,17	0.72	0
5	MAN	E	4	5	11,11,12	0.56	0	15,15,17	0.63	0
5	NAG	F	1	1,5	14,14,15	0.53	0	17,19,21	1.26	1 (5%)
5	NAG	F	2	5	14,14,15	0.57	0	17,19,21	0.75	0
5	BMA	F	3	5	11,11,12	0.56	0	15,15,17	0.56	0
5	MAN	F	4	5	11,11,12	0.59	0	15,15,17	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
5	MAN	E	4	5	-	1/2/19/22	1/1/1/1
5	NAG	F	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	2/2/19/22	1/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1	NAG	C2-N2-C7	3.25	127.25	122.90
5	E	1	NAG	C1-O5-C5	2.56	115.62	112.19

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C3-C2-N2-C7
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	F	1	NAG	C3-C2-N2-C7
5	F	4	MAN	O5-C5-C6-O6

All (2) ring outliers are listed below:

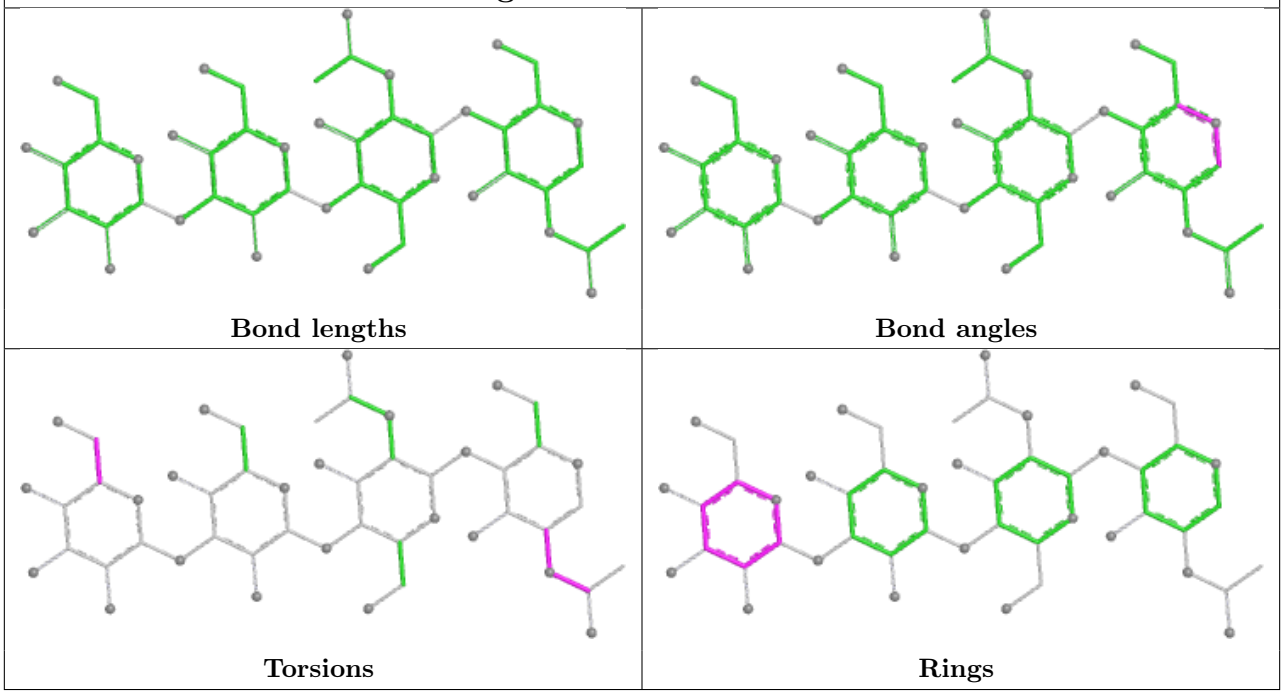
Mol	Chain	Res	Type	Atoms
5	F	4	MAN	C1-C2-C3-C4-C5-O5
5	E	4	MAN	C1-C2-C3-C4-C5-O5

4 monomers are involved in 2 short contacts:

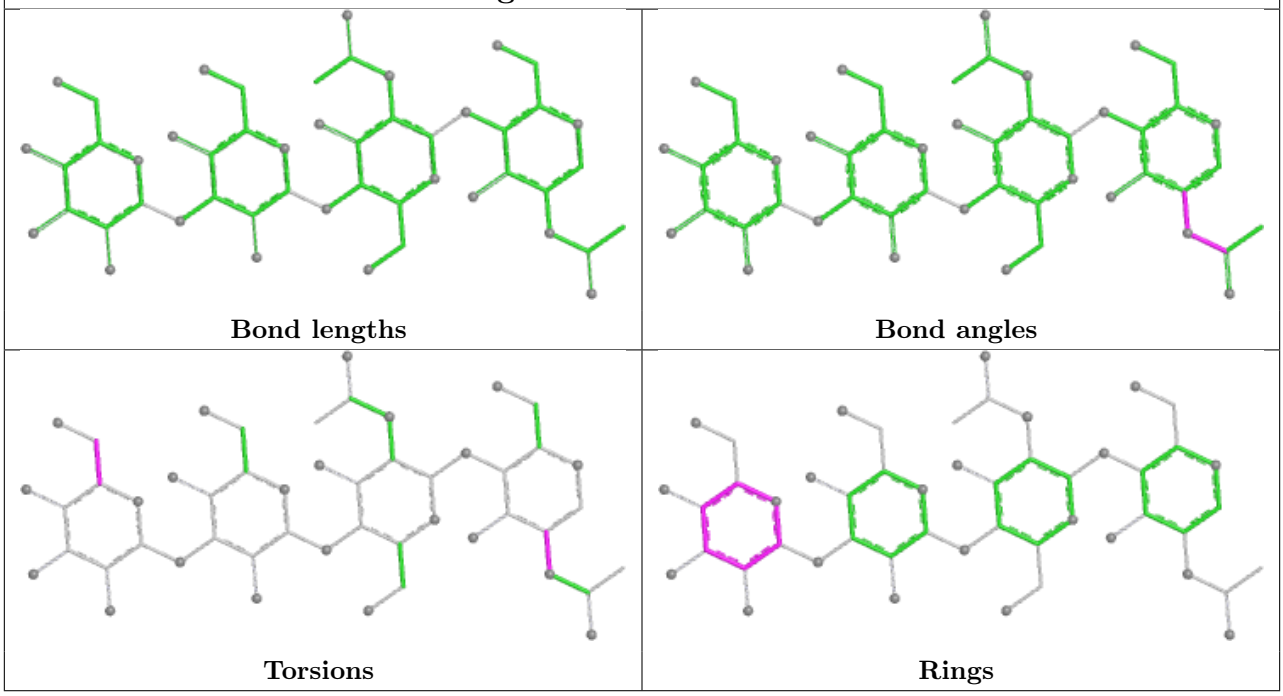
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2	NAG	1	0
5	F	4	MAN	1	0
5	F	3	BMA	1	0
5	E	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain E



Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 12 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
7	NAG	B	3415	2	14,14,15	0.53	0	17,19,21	1.18	1 (5%)
7	NAG	C	3046	1	14,14,15	0.55	0	17,19,21	0.95	1 (5%)
7	NAG	A	3447	1	14,14,15	0.45	0	17,19,21	1.13	1 (5%)
7	NAG	C	3105	1	14,14,15	0.55	0	17,19,21	0.99	2 (11%)
7	NAG	C	3447	1	14,14,15	0.54	0	17,19,21	0.57	0
7	NAG	A	3485	1	14,14,15	0.41	0	17,19,21	2.03	3 (17%)
7	NAG	A	3105	1	14,14,15	0.56	0	17,19,21	0.64	0
7	NAG	D	3260	2	14,14,15	0.57	0	17,19,21	0.74	0
8	TRS	A	598	-	7,7,7	1.42	0	9,9,9	1.54	2 (22%)
7	NAG	C	3485	1	14,14,15	0.48	0	17,19,21	2.20	5 (29%)
10	0DU	D	4000	-	37,37,37	2.30	8 (21%)	50,55,55	1.49	9 (18%)
7	NAG	B	3260	2	14,14,15	0.62	0	17,19,21	0.66	0
7	NAG	A	3046	1	14,14,15	0.56	0	17,19,21	0.77	0
10	0DU	B	4000	9	37,37,37	2.31	8 (21%)	50,55,55	1.60	9 (18%)

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
7	NAG	B	3415	2	-	5/6/23/26	0/1/1/1
7	NAG	C	3046	1	-	0/6/23/26	0/1/1/1
7	NAG	A	3447	1	-	3/6/23/26	0/1/1/1
7	NAG	C	3105	1	-	2/6/23/26	0/1/1/1
7	NAG	C	3447	1	-	2/6/23/26	0/1/1/1
7	NAG	A	3485	1	-	4/6/23/26	0/1/1/1
7	NAG	A	3105	1	-	1/6/23/26	0/1/1/1
7	NAG	D	3260	2	-	2/6/23/26	0/1/1/1
8	TRS	A	598	-	-	3/9/9/9	-
7	NAG	C	3485	1	-	4/6/23/26	0/1/1/1
10	0DU	D	4000	-	-	0/26/26/26	0/3/3/3
7	NAG	B	3260	2	-	2/6/23/26	0/1/1/1
7	NAG	A	3046	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	0DU	B	4000	9	-	0/26/26/26	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	4000	0DU	O33-C32	10.52	1.44	1.23
10	D	4000	0DU	O33-C32	10.27	1.44	1.23
10	D	4000	0DU	C17-N16	5.96	1.48	1.34
10	B	4000	0DU	C17-N16	5.57	1.47	1.34
10	B	4000	0DU	C32-N34	-3.11	1.34	1.40

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	3485	NAG	C1-O5-C5	5.73	119.87	112.19
7	A	3485	NAG	O5-C5-C6	5.63	118.62	107.66
7	C	3485	NAG	O5-C1-C2	5.43	119.69	111.29
10	B	4000	0DU	C01-C02-N34	4.44	124.23	118.52
7	A	3485	NAG	O5-C1-C2	-4.23	104.75	111.29

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	3415	NAG	C8-C7-N2-C2
7	B	3415	NAG	O7-C7-N2-C2
7	C	3447	NAG	C8-C7-N2-C2
7	C	3447	NAG	O7-C7-N2-C2
7	C	3485	NAG	C8-C7-N2-C2

There are no ring outliers.

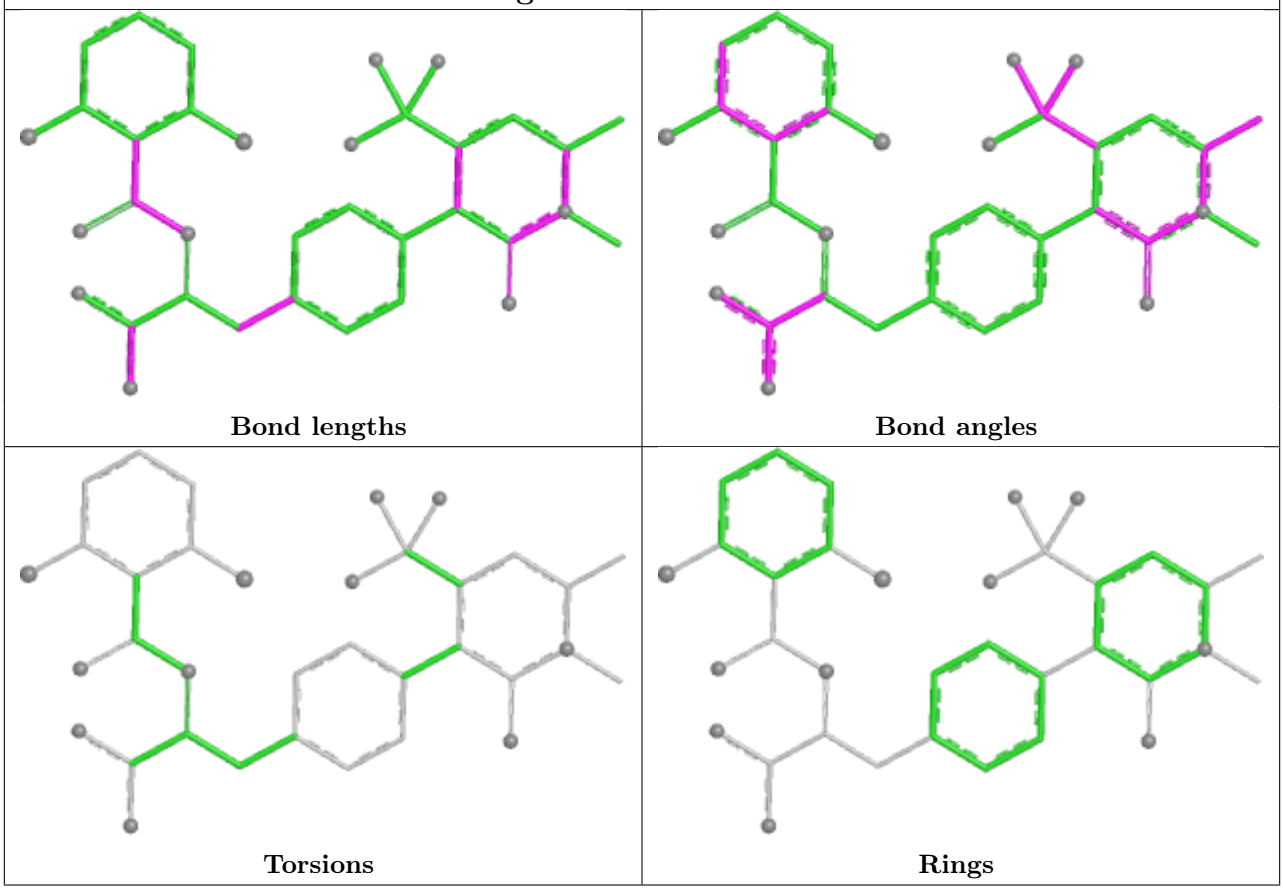
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	3415	NAG	1	0
10	D	4000	0DU	2	0
7	A	3046	NAG	1	0
10	B	4000	0DU	2	0

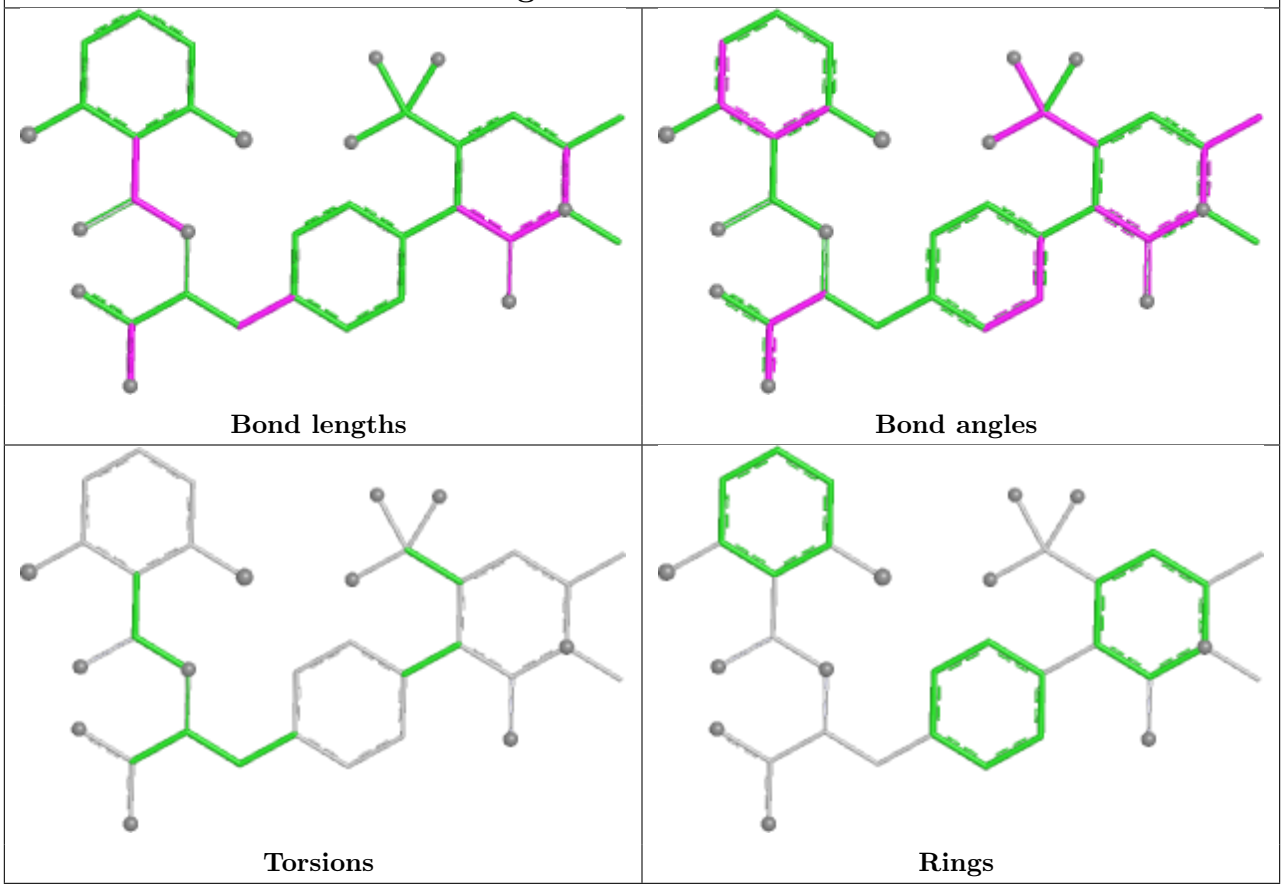
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 0DU D 4000



Ligand 0DU B 4000



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	582/597 (97%)	-0.05	5 (0%)	84	69	60, 104, 178, 229	2 (0%)
1	C	580/597 (97%)	-0.16	7 (1%)	79	61	64, 108, 188, 230	2 (0%)
2	B	375/503 (74%)	-0.08	5 (1%)	77	59	60, 110, 184, 229	0
2	D	375/503 (74%)	-0.18	6 (1%)	72	51	69, 112, 182, 231	0
3	H	211/219 (96%)	0.30	14 (6%)	18	7	67, 138, 211, 237	0
3	M	213/219 (97%)	-0.14	1 (0%)	91	81	73, 124, 192, 218	2 (0%)
4	L	217/217 (100%)	0.26	17 (7%)	13	5	74, 139, 197, 218	0
4	N	217/217 (100%)	-0.10	0	100	100	70, 119, 185, 215	0
All	All	2770/3072 (90%)	-0.06	55 (1%)	65	44	60, 114, 190, 237	6 (0%)

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	455	CYS	5.4
3	H	200	THR	4.2
3	H	132	LEU	4.0
3	H	133	ALA	3.9
2	D	99	GLU	3.8

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

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

6.3 Carbohydrates (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. The B-factors column lists the minimum,

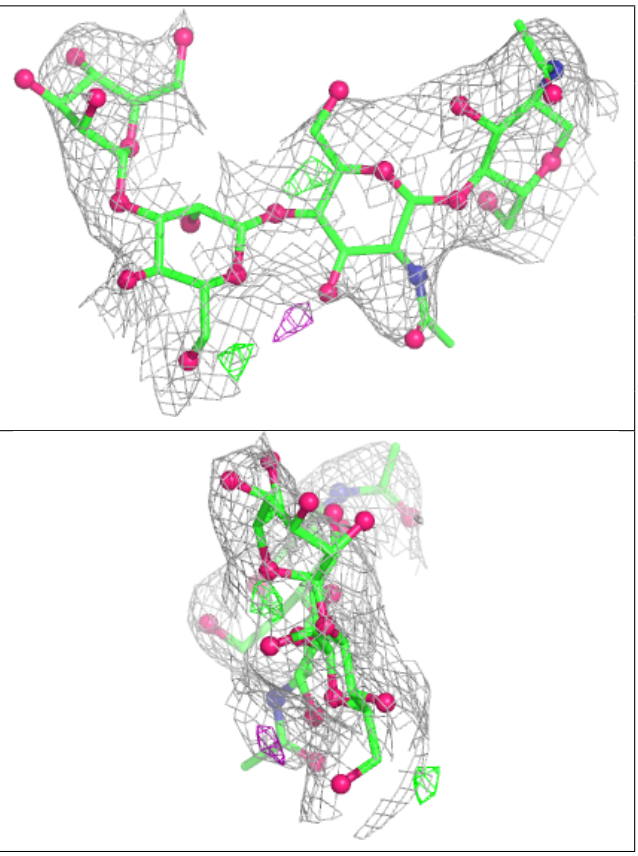
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	F	3	11/12	0.40	0.41	164,262,307,328	0
5	MAN	F	4	11/12	0.48	0.56	170,228,288,305	0
5	BMA	E	3	11/12	0.80	0.14	109,185,229,238	0
5	MAN	E	4	11/12	0.80	0.26	116,197,216,219	0
5	NAG	E	2	14/15	0.83	0.24	127,183,213,232	0
5	NAG	F	2	14/15	0.85	0.21	119,177,211,242	0
5	NAG	E	1	14/15	0.93	0.16	101,133,184,193	0
5	NAG	F	1	14/15	0.94	0.17	64,144,168,188	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

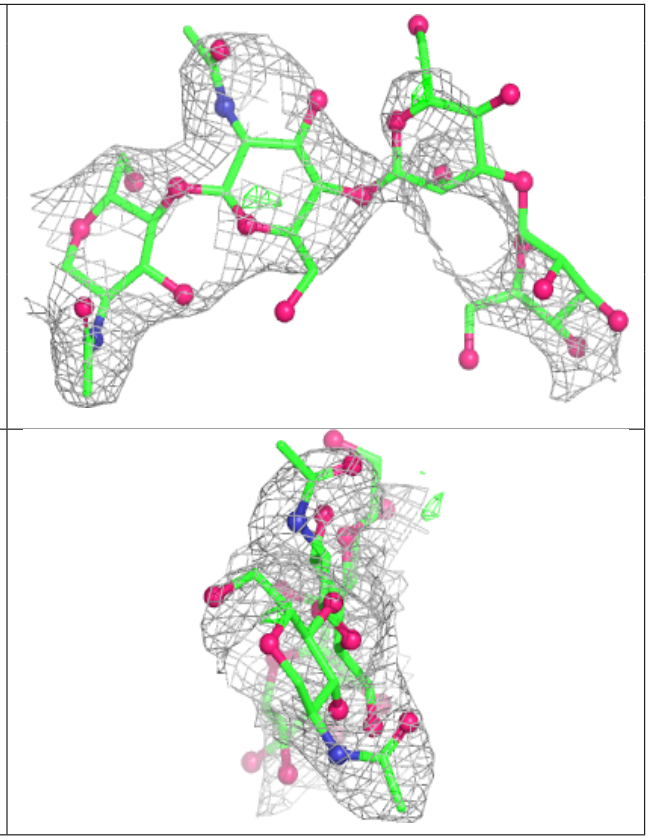
Electron density around Chain E:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain F:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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. 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	B-factors(Å^2)	Q<0.9
6	CA	B	2002	1/1	0.68	0.09	140,140,140,140	0
6	CA	C	2006	1/1	0.71	0.24	102,102,102,102	0
6	CA	D	2002	1/1	0.81	0.09	145,145,145,145	0
7	NAG	A	3485	14/15	0.83	0.31	93,177,211,223	0
7	NAG	B	3260	14/15	0.83	0.21	142,184,201,204	0
7	NAG	C	3485	14/15	0.84	0.24	153,180,207,207	0
7	NAG	A	3105	14/15	0.86	0.23	94,159,196,207	0
6	CA	A	2006	1/1	0.86	0.24	92,92,92,92	0
7	NAG	D	3260	14/15	0.87	0.19	102,175,224,228	0
7	NAG	C	3447	14/15	0.88	0.37	109,182,221,228	0
6	CA	C	2005	1/1	0.89	0.23	96,96,96,96	0
6	CA	C	2007	1/1	0.89	0.21	99,99,99,99	0
7	NAG	B	3415	14/15	0.89	0.30	112,171,206,231	0
7	NAG	C	3105	14/15	0.90	0.14	75,163,185,186	0

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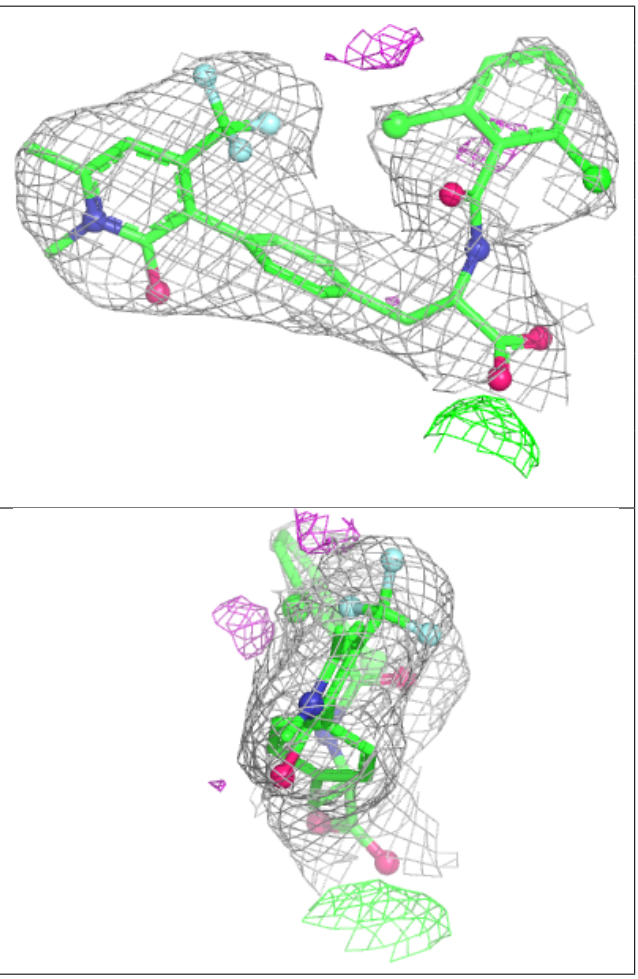
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	A	3447	14/15	0.90	0.22	102,171,199,199	0
8	TRS	A	598	8/8	0.90	0.34	80,145,172,174	0
9	MG	D	2001	1/1	0.92	0.19	61,61,61,61	0
6	CA	B	2003	1/1	0.94	0.26	69,69,69,69	0
7	NAG	A	3046	14/15	0.95	0.15	78,103,135,141	0
9	MG	B	2001	1/1	0.95	0.23	49,49,49,49	0
6	CA	A	2005	1/1	0.95	0.30	86,86,86,86	0
7	NAG	C	3046	14/15	0.96	0.17	83,118,139,161	0
6	CA	D	2003	1/1	0.96	0.23	83,83,83,83	0
10	0DU	D	4000	35/35	0.96	0.27	55,119,193,221	0
10	0DU	B	4000	35/35	0.97	0.22	46,96,152,165	0
6	CA	A	2007	1/1	0.97	0.23	79,79,79,79	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

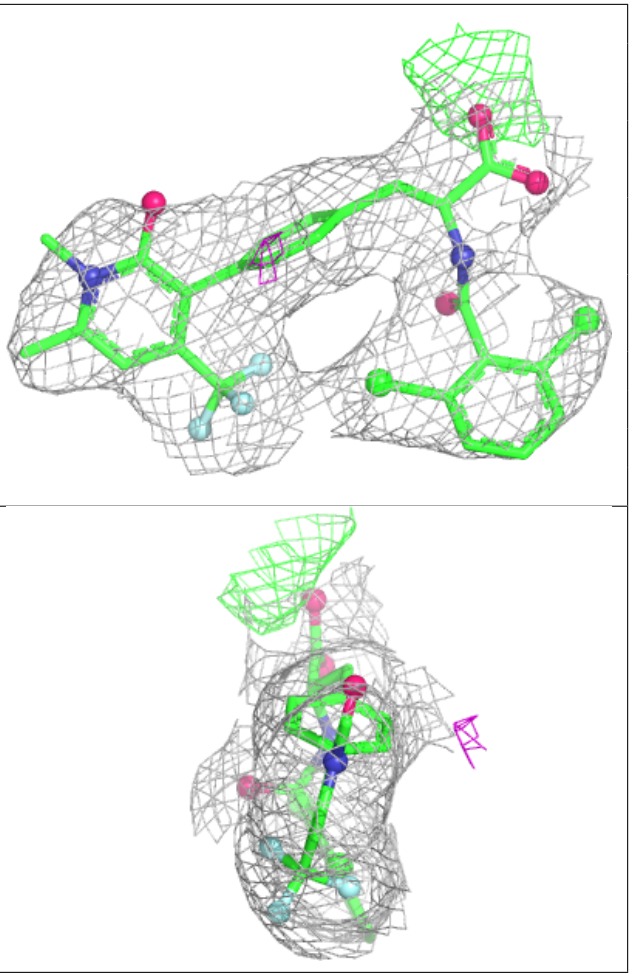
Electron density around 0DU D 4000:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 0DU B 4000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.