



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:48 AM GMT

PDB ID : 2IQ7  
Title : Crystal structure of the polygalacturonase from Colletotrichum lupini and its implications for the interaction with polygalacturonase-inhibiting proteins  
Authors : Bonivento, D.; Federici, L.; Matteo, A.D.  
Deposited on : 2006-10-13  
Resolution : 1.94 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](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

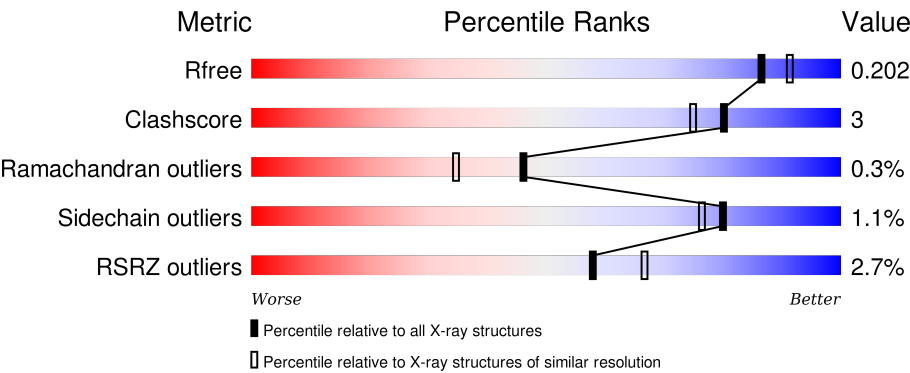
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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 <=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	339	<div><div></div><div>94%5%•</div></div>
1	B	339	<div><div>%</div><div>92%8%</div></div>
1	C	339	<div><div></div><div>92%7%•</div></div>
1	D	339	<div><div></div><div>92%8%</div></div>
1	E	339	<div><div></div><div>91%8%•</div></div>

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Mol	Chain	Length	Quality of chain
1	F	339	
1	G	339	

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	MAN	H	365	X	-	-	-
2	MAN	H	368	-	-	-	X
3	NAG	L	363	-	-	-	X
3	NAG	M	363	-	-	-	X
3	NAG	O	363	-	-	-	X
3	NAG	Q	363	-	-	-	X
4	PG4	A	3004	-	-	-	X
4	PG4	D	3006	-	-	-	X
4	PG4	E	3001	-	-	-	X
4	PG4	F	3005	-	-	-	X
5	PEG	B	3008	-	-	-	X
5	PEG	E	3007	-	-	-	X
5	PEG	F	3009	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 19675 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 endopolygalacturonase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	3	0
			2412	1486	413	503	10			
1	B	339	Total	C	N	O	S	0	5	0
			2419	1493	413	503	10			
1	C	339	Total	C	N	O	S	0	4	0
			2416	1490	414	502	10			
1	D	339	Total	C	N	O	S	0	4	0
			2419	1492	416	501	10			
1	E	339	Total	C	N	O	S	0	9	0
			2439	1504	417	508	10			
1	F	338	Total	C	N	O	S	0	3	0
			2406	1482	412	502	10			
1	G	339	Total	C	N	O	S	0	2	0
			2404	1481	412	501	10			

- Molecule 2 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	6	Total	C	N	O	0	0
			72	40	2	30		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



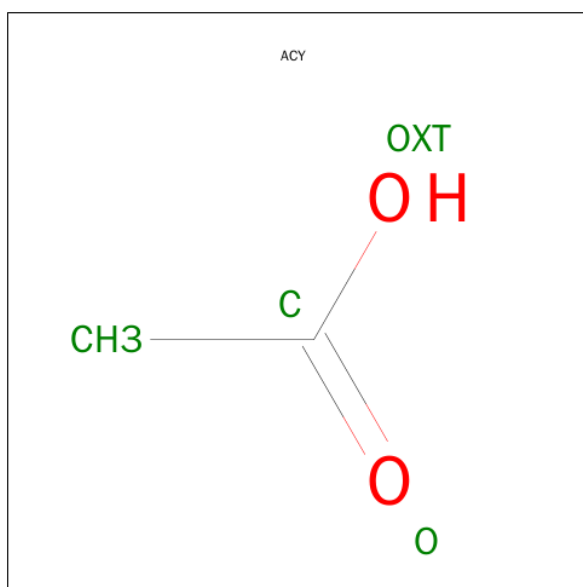
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			11	7	4		
4	A	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			6	4	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	367	Total O 367 367	0	0
7	B	361	Total O 361 361	0	0
7	C	413	Total O 413 413	0	0
7	D	352	Total O 352 352	0	0
7	E	374	Total O 374 374	0	0
7	F	316	Total O 316 316	0	0
7	G	206	Total O 206 206	0	0
7	H	19	Total O 19 19	0	0
7	I	6	Total O 6 6	0	0
7	L	4	Total O 4 4	0	0
7	M	5	Total O 5 5	0	0
7	N	8	Total O 8 8	0	0
7	O	3	Total O 3 3	0	0
7	Q	4	Total O 4 4	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: endopolygalacturonase

Chain A: 



- Molecule 1: endopolygalacturonase

Chain B: 



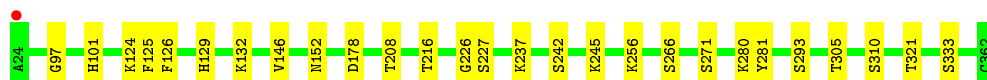
- Molecule 1: endopolygalacturonase

Chain C: 



- Molecule 1: endopolygalacturonase

Chain D: 



- Molecule 1: endopolygalacturonase

Chain E: 



- Molecule 1: endopolygalacturonase

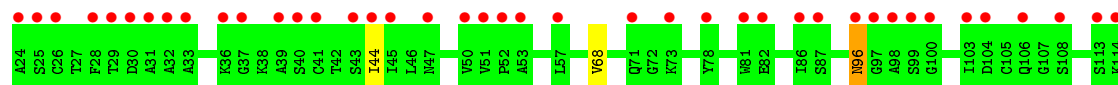
Chain F: 





- Molecule 1: endopolygalacturonase

Chain G: 17% 92% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.64Å 127.27Å 205.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.33 – 1.94 49.35 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.33-1.94) 99.0 (49.35-1.94)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.44 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.152 , 0.196 0.168 , 0.202	Depositor DCC
$R_{free}$ test set	8252 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 164243 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19675	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.56% 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: ACY, PG4, PEG, NAG, MAN

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	0.55	0/2459	0.61	0/3338
1	B	0.55	0/2472	0.62	0/3356
1	C	0.56	0/2466	0.62	0/3346
1	D	0.50	0/2470	0.60	0/3351
1	E	0.55	0/2504	0.62	0/3397
1	F	0.50	0/2453	0.59	0/3329
1	G	0.46	0/2448	0.56	0/3322
All	All	0.53	0/17272	0.60	0/23439

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	365	MAN	C1

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	2412	0	2363	15	0
1	B	2419	0	2382	15	0
1	C	2416	0	2377	15	0
1	D	2419	0	2377	16	0
1	E	2439	0	2404	22	0
1	F	2406	0	2356	16	0
1	G	2404	0	2356	16	0
2	H	72	0	61	3	0
3	I	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	1	0
3	O	28	0	25	0	0
3	Q	28	0	25	0	0
4	A	7	0	9	0	0
4	B	11	0	13	1	0
4	C	10	0	13	1	0
4	D	6	0	7	0	0
4	E	10	0	13	2	0
4	F	13	0	18	5	0
5	B	7	0	10	2	0
5	E	7	0	10	3	0
5	F	7	0	10	1	0
6	B	4	0	3	0	0
7	A	367	0	0	2	0
7	B	361	0	0	2	0
7	C	413	0	0	2	0
7	D	352	0	0	3	0
7	E	374	0	0	1	0
7	F	316	0	0	1	0
7	G	206	0	0	2	0
7	H	19	0	0	0	0
7	I	6	0	0	0	0
7	L	4	0	0	0	0
7	M	5	0	0	0	0
7	N	8	0	0	0	0
7	O	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Q	4	0	0	0	0
All	All	19675	0	16932	117	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.

The worst 5 of 117 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:E:42:THR:HG22	1:E:63:LYS:HZ1	1.27	0.97
1:E:306:GLY:HA3	4:E:3001:PG4:H51	1.48	0.95
1:E:42:THR:HG22	1:E:63:LYS:NZ	1.88	0.88
1:F:109:ARG:HA	4:F:3005:PG4:H22	1.60	0.82
1:F:109:ARG:HH11	4:F:3005:PG4:H82	1.47	0.79

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	340/339 (100%)	326 (96%)	13 (4%)	1 (0%)	46	35
1	B	342/339 (101%)	328 (96%)	13 (4%)	1 (0%)	46	35
1	C	341/339 (101%)	330 (97%)	10 (3%)	1 (0%)	46	35
1	D	341/339 (101%)	326 (96%)	14 (4%)	1 (0%)	46	35
1	E	346/339 (102%)	331 (96%)	14 (4%)	1 (0%)	46	35
1	F	339/339 (100%)	328 (97%)	10 (3%)	1 (0%)	46	35
1	G	339/339 (100%)	325 (96%)	13 (4%)	1 (0%)	46	35
All	All	2388/2373 (101%)	2294 (96%)	87 (4%)	7 (0%)	46	35

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	VAL
1	B	146	VAL
1	D	146	VAL
1	E	146	VAL
1	F	146	VAL

### 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	269/266 (101%)	266 (99%)	3 (1%)	80	76
1	B	271/266 (102%)	267 (98%)	4 (2%)	72	66
1	C	270/266 (102%)	267 (99%)	3 (1%)	80	76
1	D	270/266 (102%)	268 (99%)	2 (1%)	88	87
1	E	275/266 (103%)	271 (98%)	4 (2%)	72	66
1	F	269/266 (101%)	267 (99%)	2 (1%)	88	87
1	G	268/266 (101%)	265 (99%)	3 (1%)	80	76
All	All	1892/1862 (102%)	1871 (99%)	21 (1%)	80	76

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	146	VAL
1	D	293	SER
1	F	178	ASP
1	C	132	LYS
1	G	96	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	277	ASN

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Mol	Chain	Res	Type
1	D	71	GLN
1	F	277	ASN
1	C	117	ASN
1	G	96	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

18 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	NAG	H	363	1,2	14,14,15	0.62	0	15,19,21	0.86	0
2	NAG	H	364	2	14,14,15	0.54	0	15,19,21	0.92	1 (6%)
2	MAN	H	365	2	11,11,12	0.71	0	14,15,17	0.95	0
2	MAN	H	366	2	11,11,12	0.59	0	14,15,17	1.23	1 (7%)
2	MAN	H	367	2	11,11,12	0.51	0	14,15,17	1.04	1 (7%)
2	MAN	H	368	2	11,11,12	0.58	0	14,15,17	1.50	3 (21%)
3	NAG	I	363	1,3	14,14,15	0.54	0	15,19,21	0.74	0
3	NAG	I	364	3	14,14,15	0.45	0	15,19,21	1.12	1 (6%)
3	NAG	L	363	1,3	14,14,15	0.59	0	15,19,21	0.68	0
3	NAG	L	364	3	14,14,15	0.37	0	15,19,21	1.48	1 (6%)
3	NAG	M	363	1,3	14,14,15	0.61	0	15,19,21	1.01	1 (6%)
3	NAG	M	364	3	14,14,15	0.58	0	15,19,21	0.79	1 (6%)
3	NAG	N	363	1,3	14,14,15	0.62	0	15,19,21	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	N	364	3	14,14,15	0.49	0	15,19,21	1.20	1 (6%)
3	NAG	O	363	1,3	14,14,15	0.65	0	15,19,21	1.04	0
3	NAG	O	364	3	14,14,15	0.48	0	15,19,21	1.52	1 (6%)
3	NAG	Q	363	1,3	14,14,15	0.61	0	15,19,21	0.87	0
3	NAG	Q	364	3	14,14,15	0.50	0	15,19,21	1.25	1 (6%)

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	NAG	H	363	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	364	2	-	0/6/23/26	0/1/1/1
2	MAN	H	365	2	1/1/4/5	0/2/19/22	0/1/1/1
2	MAN	H	366	2	-	0/2/19/22	0/1/1/1
2	MAN	H	367	2	-	0/2/19/22	0/1/1/1
2	MAN	H	368	2	-	0/2/19/22	0/1/1/1
3	NAG	I	363	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	364	3	-	0/6/23/26	0/1/1/1
3	NAG	L	363	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	364	3	-	0/6/23/26	0/1/1/1
3	NAG	M	363	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	364	3	-	0/6/23/26	0/1/1/1
3	NAG	N	363	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	364	3	-	0/6/23/26	0/1/1/1
3	NAG	O	363	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	364	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	363	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Q	364	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	367	MAN	O5-C1-C2	-2.20	107.29	110.86
3	M	364	NAG	C1-O5-C5	2.05	114.85	112.25
2	H	368	MAN	C1-C2-C3	2.11	112.04	109.54
2	H	366	MAN	O5-C1-C2	2.15	114.34	110.86
2	H	368	MAN	O5-C1-C2	2.20	114.42	110.86



All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	365	MAN	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	363	NAG	1	0
2	H	367	MAN	2	0
3	N	363	NAG	1	0

## 5.6 Ligand geometry [i](#)

10 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	$\# Z  > 2$
4	PG4	A	3004	-	6,6,12	0.40	0	5,5,11	0.42	0
4	PG4	B	3003	-	10,10,12	0.47	0	9,9,11	0.29	0
5	PEG	B	3008	-	6,6,6	0.46	0	5,5,5	0.24	0
6	ACY	B	3010	-	1,3,3	1.30	0	0,3,3	0.00	-
4	PG4	C	3002	-	9,9,12	0.47	0	8,8,11	0.40	0
4	PG4	D	3006	-	5,5,12	0.50	0	4,4,11	0.27	0
4	PG4	E	3001	-	9,9,12	0.57	0	8,8,11	0.49	0
5	PEG	E	3007	-	6,6,6	0.43	0	5,5,5	0.57	0
4	PG4	F	3005	-	12,12,12	0.48	0	11,11,11	0.32	0
5	PEG	F	3009	-	6,6,6	0.47	0	5,5,5	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	A	3004	-	-	0/4/4/10	0/0/0/0
4	PG4	B	3003	-	-	0/8/8/10	0/0/0/0
5	PEG	B	3008	-	-	0/4/4/4	0/0/0/0
6	ACY	B	3010	-	-	0/0/0/0	0/0/0/0
4	PG4	C	3002	-	-	0/7/7/10	0/0/0/0
4	PG4	D	3006	-	-	0/3/3/10	0/0/0/0
4	PG4	E	3001	-	-	0/7/7/10	0/0/0/0
5	PEG	E	3007	-	-	0/4/4/4	0/0/0/0
4	PG4	F	3005	-	-	0/10/10/10	0/0/0/0
5	PEG	F	3009	-	-	0/4/4/4	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.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3003	PG4	1	0
5	B	3008	PEG	2	0
4	C	3002	PG4	1	0
4	E	3001	PG4	2	0
5	E	3007	PEG	3	0
4	F	3005	PG4	5	0
5	F	3009	PEG	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 [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, 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	339/339 (100%)	-0.24	0 100 100	6, 9, 18, 28	0
1	B	339/339 (100%)	0.01	3 (0%) 85 89	6, 9, 17, 26	0
1	C	339/339 (100%)	-0.30	0 100 100	5, 9, 16, 27	0
1	D	339/339 (100%)	-0.21	1 (0%) 94 96	8, 12, 19, 32	0
1	E	339/339 (100%)	-0.23	0 100 100	6, 9, 15, 26	0
1	F	338/339 (99%)	-0.11	3 (0%) 85 89	9, 12, 19, 26	0
1	G	339/339 (100%)	1.01	58 (17%) 2 3	16, 21, 30, 36	0
All	All	2372/2373 (99%)	-0.01	65 (2%) 58 67	5, 11, 23, 36	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	24	ALA	4.6
1	G	39	ALA	4.4
1	G	26	CYS	4.3
1	G	71	GLN	4.1
1	G	25	SER	4.1

### 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. 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
3	NAG	O	363	14/15	0.95	0.17	24.46	13,17,22,22	0
3	NAG	M	363	14/15	0.94	0.12	4.76	17,20,23,24	0
2	MAN	H	368	11/12	0.81	0.18	3.78	34,36,37,38	0
3	NAG	Q	363	14/15	0.89	0.16	3.12	24,26,29,29	0
3	NAG	L	363	14/15	0.94	0.10	2.99	17,21,25,26	0
2	MAN	H	366	11/12	0.89	0.12	1.39	16,17,21,21	0
3	NAG	N	363	14/15	0.95	0.10	0.61	11,14,17,19	0
3	NAG	I	363	14/15	0.93	0.10	0.06	13,17,21,22	0
2	MAN	H	365	11/12	0.97	0.10	-0.04	11,13,15,22	0
2	NAG	H	363	14/15	0.97	0.09	-0.16	6,9,17,17	0
3	NAG	M	364	14/15	0.94	0.11	-	22,24,26,27	0
3	NAG	O	364	14/15	0.91	0.20	-	24,25,29,30	0
3	NAG	I	364	14/15	0.88	0.20	-	21,26,30,31	0
3	NAG	L	364	14/15	0.87	0.21	-	30,35,39,40	0
3	NAG	N	364	14/15	0.95	0.09	-	18,21,23,25	0
3	NAG	Q	364	14/15	0.89	0.18	-	30,32,35,37	0
2	MAN	H	367	11/12	0.79	0.21	-	30,35,37,40	0
2	NAG	H	364	14/15	0.96	0.09	-	8,11,12,13	0

## 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
5	PEG	B	3008	7/7	0.70	0.23	12.38	46,46,47,48	0
4	PG4	E	3001	10/13	0.75	0.24	9.16	22,26,27,29	0
5	PEG	E	3007	7/7	0.82	0.18	6.27	28,30,32,32	0
4	PG4	A	3004	7/13	0.93	0.12	4.86	27,28,30,30	0
4	PG4	F	3005	13/13	0.77	0.19	3.86	31,35,39,39	0
5	PEG	F	3009	7/7	0.74	0.23	3.71	38,40,43,43	0
4	PG4	D	3006	6/13	0.81	0.18	2.02	43,45,47,47	0
4	PG4	B	3003	11/13	0.89	0.15	1.80	33,35,36,37	0
6	ACY	B	3010	4/4	0.86	0.16	1.48	30,30,30,31	0
4	PG4	C	3002	10/13	0.85	0.14	0.97	33,35,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.