



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 11:17 PM BST

PDB ID : 4UI2  
Title : Crystal structure of the ternary RGMB-BMP2-NEO1 complex  
Authors : Healey, E.G.; Bishop, B.; Elegheert, J.; Bell, C.H.; Padilla-Parra, S.; Siebold, C.  
Deposited on : 2015-03-27  
Resolution : 3.15 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

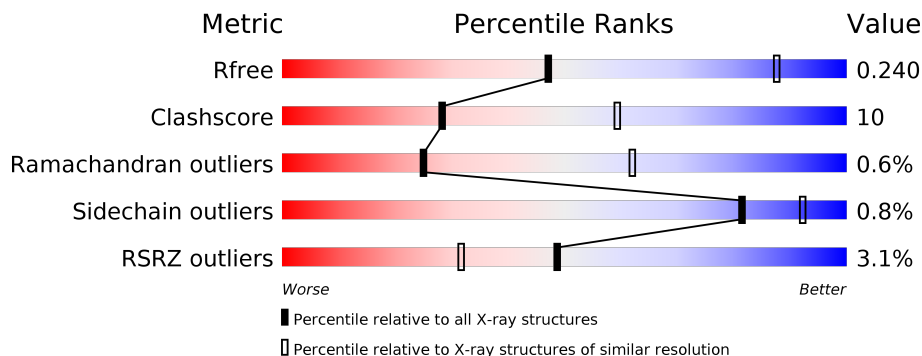
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 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  $\leq 5\%$ . 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	264	 2% 66% 9% 24%
2	B	114	 4% 71% 19% 9%
3	C	122	 2% 56% 9% 34%
4	D	251	 2% 47% 14% 38%
5	E	3	 100%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
6	SRT	B	1399	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4311 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 NEOGENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	201	1596	1018	274	298	6	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	880	GLU	-	expression tag	UNP P97798
A	881	THR	-	expression tag	UNP P97798
A	882	GLY	-	expression tag	UNP P97798
A	1134	ASN	-	expression tag	UNP P97798
A	1135	GLY	-	expression tag	UNP P97798
A	1136	THR	-	expression tag	UNP P97798
A	1137	LYS	-	expression tag	UNP P97798
A	1138	HIS	-	expression tag	UNP P97798
A	1139	HIS	-	expression tag	UNP P97798
A	1140	HIS	-	expression tag	UNP P97798
A	1141	HIS	-	expression tag	UNP P97798
A	1142	HIS	-	expression tag	UNP P97798
A	1143	HIS	-	expression tag	UNP P97798

- Molecule 2 is a protein called BONE MORPHOGENETIC PROTEIN 2, BMP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	104	814	516	137	152	9	0	0	0

- Molecule 3 is a protein called REPULSIVE GUIDANCE MOLECULE C, RGMC, HEMO-JUVELIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	80	616	378	111	118	9	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	47	GLU	-	expression tag	UNP Q6NW40
C	48	THR	-	expression tag	UNP Q6NW40
C	49	GLY	-	expression tag	UNP Q6NW40

- Molecule 4 is a protein called REPULSIVE GUIDANCE MOLECULE C, RGMC, HEMO-JUVELIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	156	1212	757	210	238	7	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

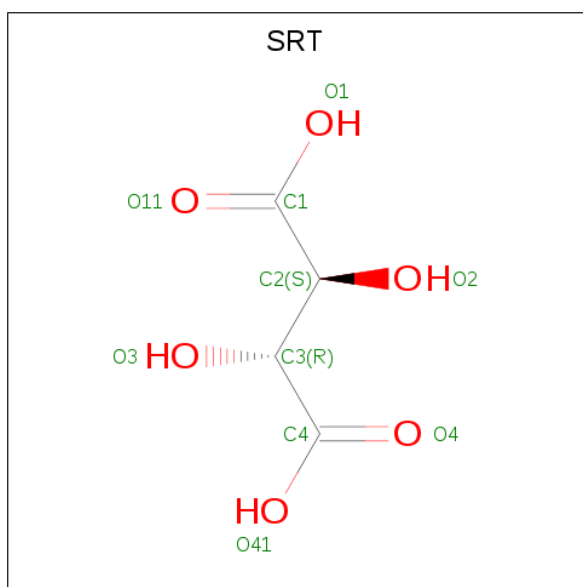
Chain	Residue	Modelled	Actual	Comment	Reference
D	411	GLY	-	expression tag	UNP Q6NW40
D	412	THR	-	expression tag	UNP Q6NW40
D	413	LYS	-	expression tag	UNP Q6NW40
D	414	HIS	-	expression tag	UNP Q6NW40
D	415	HIS	-	expression tag	UNP Q6NW40
D	416	HIS	-	expression tag	UNP Q6NW40
D	417	HIS	-	expression tag	UNP Q6NW40
D	418	HIS	-	expression tag	UNP Q6NW40
D	419	HIS	-	expression tag	UNP Q6NW40
D	225	GLY	GLU	conflict	UNP Q6NW40

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



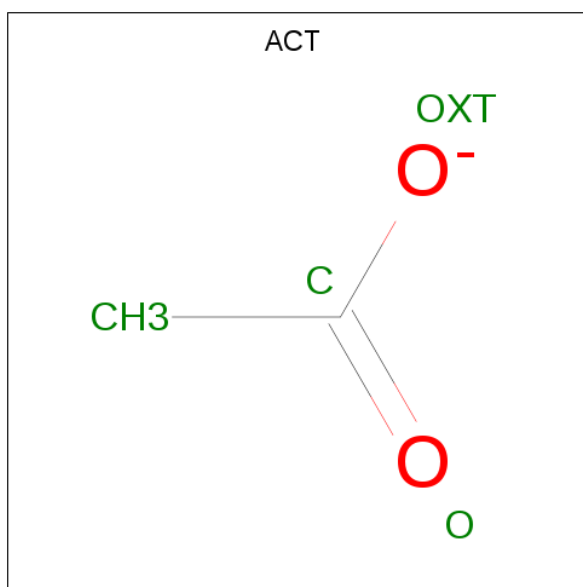
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	3	39	22	2	15	0	0	0

- Molecule 6 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	4	6		
6	B	1	Total	C	O	0	0
			10	4	6		
6	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub><sup>-</sup>).

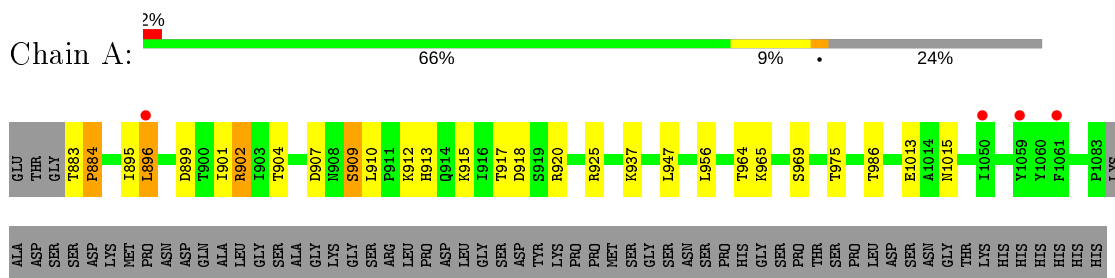


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		

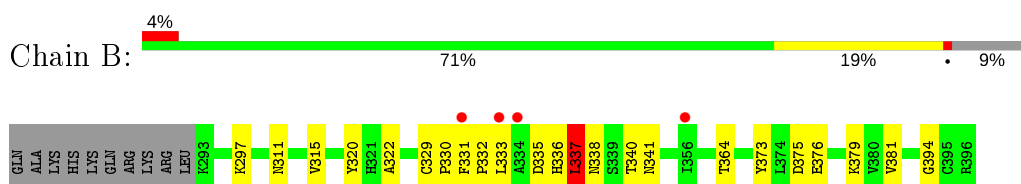
### 3 Residue-property plots [i](#)

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.

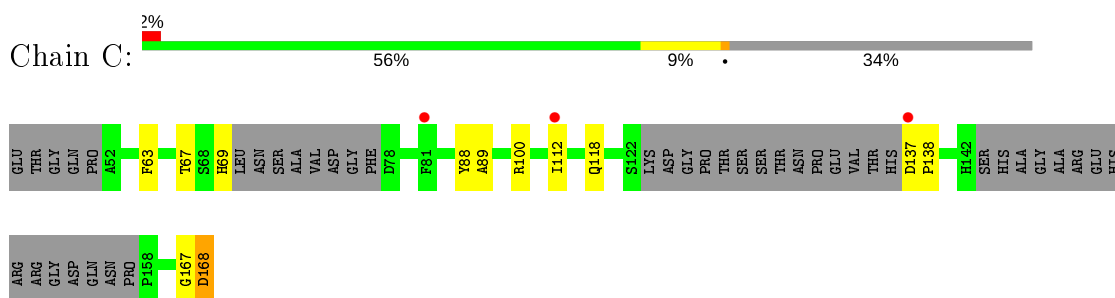
- Molecule 1: NEOGENIN



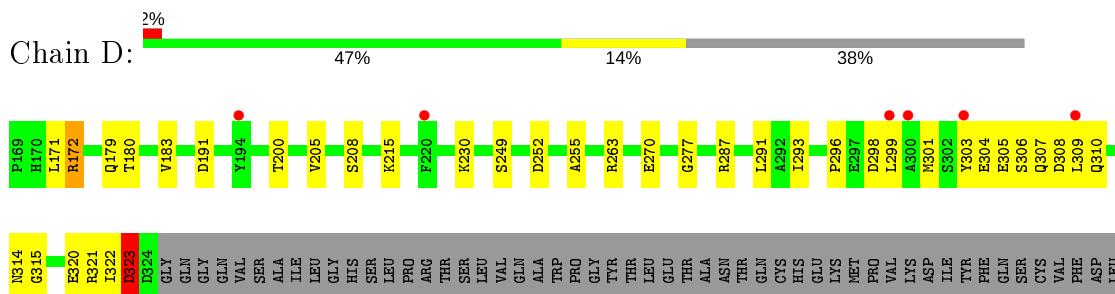
- Molecule 2: BONE MORPHOGENETIC PROTEIN 2, BMP2



- Molecule 3: REPULSIVE GUIDANCE MOLECULE C, RGMC, HEMOJUVELIN



- Molecule 4: REPULSIVE GUIDANCE MOLECULE C, RGMC, HEMOJUVELIN



LEU  
THR  
THR  
GLY  
ASP  
ALA  
ASN  
PHE  
THR  
ALA  
ALA  
ALA  
HIS  
SER  
SER  
ALA  
LEU  
GLU  
ASP  
VAL  
GLU  
ALA  
LEU  
HIS  
PRO  
ARG  
LYS  
GLU  
ARG  
TRP  
HIS  
ILE  
PHE  
PRO  
SER  
GLY  
THR  
LYS  
HIS  
HIS  
HIS  
HIS  
HIS

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

Chain E:

100%

IMAG1  
IMAG2  
BMA3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.08Å 120.08Å 204.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.15 103.50 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.01-3.15) 98.5 (103.50-3.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 3.13Å)	Xtrriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.196 , 0.236 0.203 , 0.240	Depositor DCC
$R_{free}$ test set	1302 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	107.9	Xtrriage
Anisotropy	0.695	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 109.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4311	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	135.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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, 0.333 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: BMA, NAG, SRT, ACT

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	0.62	0/1640	0.84	3/2241 (0.1%)
2	B	0.69	0/837	0.86	2/1140 (0.2%)
3	C	0.58	0/625	0.86	2/835 (0.2%)
4	D	0.64	0/1236	0.89	4/1680 (0.2%)
All	All	0.63	0/4338	0.86	11/5896 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	168	ASP	CB-CG-OD2	-9.23	109.99	118.30
1	A	896	LEU	CB-CG-CD1	8.96	126.22	111.00
4	D	323	ASP	CB-CG-OD2	6.66	124.29	118.30
4	D	172	ARG	NE-CZ-NH1	6.63	123.61	120.30
2	B	337	LEU	CA-CB-CG	5.43	127.79	115.30
3	C	168	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	902	ARG	CB-CA-C	-5.24	99.93	110.40
4	D	287	ARG	NE-CZ-NH1	5.16	122.88	120.30
4	D	323	ASP	CB-CG-OD1	-5.06	113.74	118.30
2	B	297	LYS	CD-CE-NZ	5.05	123.31	111.70
1	A	899	ASP	CB-CG-OD1	5.03	122.83	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	1596	0	1594	19	0
2	B	814	0	775	27	0
3	C	616	0	576	8	0
4	D	1212	0	1176	32	0
5	E	39	0	32	0	0
6	B	30	0	12	0	0
7	B	4	0	3	0	0
All	All	4311	0	4168	83	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 10.

All (83) 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)
2:B:332:PRO:HA	2:B:335:ASP:OD2	1.16	1.26
2:B:332:PRO:CA	2:B:335:ASP:OD2	1.92	1.15
4:D:305:GLU:OE1	4:D:306:SER:N	2.14	0.81
2:B:337:LEU:CG	2:B:338:ASN:HA	2.11	0.81
2:B:337:LEU:HG	2:B:338:ASN:HA	1.61	0.80
4:D:180:THR:HG22	4:D:322:ILE:HD12	1.66	0.77
1:A:896:LEU:HD11	1:A:902:ARG:HG3	1.67	0.76
4:D:304:GLU:O	4:D:307:GLN:HB3	1.85	0.76
4:D:301:MET:HA	4:D:303:TYR:HE1	1.52	0.73
2:B:332:PRO:C	2:B:335:ASP:OD2	2.22	0.71
4:D:191:ASP:C	4:D:310:GLN:NE2	2.44	0.70
4:D:301:MET:HA	4:D:303:TYR:CE1	2.26	0.70
2:B:329:CYS:N	2:B:330:PRO:HD3	2.05	0.70
1:A:910:LEU:HD23	1:A:915:LYS:O	1.94	0.67
4:D:323:ASP:OD1	4:D:323:ASP:N	2.26	0.67
2:B:337:LEU:CD2	2:B:338:ASN:HA	2.24	0.67
4:D:308:ASP:O	4:D:314:ASN:ND2	2.29	0.65
1:A:896:LEU:CD1	1:A:902:ARG:HG3	2.26	0.64
2:B:337:LEU:HD23	2:B:338:ASN:HA	1.79	0.64
4:D:191:ASP:O	4:D:310:GLN:NE2	2.30	0.63
2:B:337:LEU:HD23	2:B:338:ASN:CA	2.31	0.61
4:D:305:GLU:O	4:D:306:SER:OG	2.13	0.61
4:D:252:ASP:HB3	4:D:255:ALA:HB3	1.82	0.60
4:D:263:ARG:NH1	4:D:270:GLU:OE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:ARG:NH2	2:B:315:VAL:O	2.34	0.59
1:A:910:LEU:HD11	1:A:920:ARG:CZ	2.32	0.58
3:C:67:THR:O	3:C:69:HIS:ND1	2.34	0.58
4:D:304:GLU:O	4:D:307:GLN:CB	2.54	0.56
4:D:308:ASP:OD1	4:D:309:LEU:N	2.41	0.54
4:D:191:ASP:H	4:D:310:GLN:NE2	2.07	0.53
1:A:912:LYS:HG3	1:A:913:HIS:CD2	2.44	0.52
1:A:902:ARG:HG2	1:A:947:LEU:CD1	2.40	0.51
1:A:902:ARG:HG2	1:A:947:LEU:HD13	1.93	0.51
4:D:305:GLU:C	4:D:307:GLN:H	2.13	0.51
2:B:375:ASP:OD2	2:B:379:LYS:HB2	2.11	0.51
3:C:167:GLY:O	3:C:168:ASP:CB	2.59	0.51
2:B:336:HIS:O	2:B:337:LEU:HB3	2.11	0.50
2:B:338:ASN:N	2:B:338:ASN:OD1	2.42	0.50
4:D:179:GLN:HE22	4:D:315:GLY:HA3	1.76	0.50
4:D:298:ASP:OD1	4:D:299:LEU:N	2.45	0.49
4:D:180:THR:CG2	4:D:322:ILE:HD12	2.40	0.49
2:B:364:THR:HG21	2:B:394:GLY:HA3	1.94	0.48
4:D:191:ASP:N	4:D:310:GLN:NE2	2.61	0.48
4:D:183:VAL:H	4:D:320:GLU:HG3	1.79	0.48
1:A:895:ILE:HG22	1:A:901:ILE:HG12	1.96	0.48
1:A:964:THR:HA	1:A:969:SER:HA	1.95	0.47
2:B:333:LEU:O	2:B:336:HIS:HB3	2.15	0.47
2:B:337:LEU:HA	2:B:338:ASN:C	2.35	0.47
4:D:321:ARG:HG2	4:D:321:ARG:HH11	1.80	0.46
1:A:904:THR:HG21	2:B:311:ASN:ND2	2.30	0.46
2:B:336:HIS:HD2	2:B:337:LEU:O	1.98	0.46
4:D:191:ASP:C	4:D:310:GLN:HE21	2.15	0.46
1:A:925:ARG:HA	1:A:937:LYS:O	2.16	0.45
4:D:230:LYS:HE3	4:D:249:SER:O	2.16	0.45
2:B:335:ASP:OD1	2:B:336:HIS:N	2.50	0.45
4:D:205:VAL:HG22	4:D:208:SER:HB2	1.99	0.45
3:C:89:ALA:HB2	3:C:112:ILE:HG21	1.99	0.45
3:C:167:GLY:O	3:C:168:ASP:HB2	2.15	0.45
4:D:171:LEU:HD12	4:D:172:ARG:N	2.32	0.44
3:C:137:ASP:N	3:C:138:PRO:CD	2.81	0.44
4:D:191:ASP:HB3	4:D:310:GLN:HE21	1.82	0.44
4:D:291:LEU:HD21	4:D:293:ILE:HD11	1.99	0.44
2:B:320:TYR:CZ	2:B:322:ALA:HB2	2.54	0.43
4:D:191:ASP:CA	4:D:310:GLN:NE2	2.82	0.43
2:B:375:ASP:O	3:C:100:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:200:THR:HB	4:D:215:LYS:HB3	2.00	0.43
1:A:915:LYS:HG2	1:A:917:THR:OG1	2.18	0.43
2:B:331:PHE:N	2:B:331:PHE:CD1	2.87	0.43
1:A:883:THR:OG1	1:A:884:PRO:HD3	2.19	0.43
2:B:340:THR:O	2:B:341:ASN:C	2.58	0.42
2:B:329:CYS:N	2:B:330:PRO:CD	2.77	0.42
2:B:373:TYR:CZ	2:B:381:VAL:HG11	2.55	0.42
1:A:907:ASP:OD1	1:A:909:SER:HB2	2.20	0.42
2:B:376:GLU:HA	2:B:376:GLU:OE1	2.20	0.42
1:A:918:ASP:OD2	1:A:965:LYS:HE2	2.19	0.42
3:C:118:GLN:O	3:C:118:GLN:HG3	2.20	0.42
1:A:986:THR:HG23	1:A:1015:ASN:ND2	2.34	0.41
3:C:63:PHE:CD1	3:C:88:TYR:HB2	2.55	0.41
1:A:917:THR:HG22	1:A:917:THR:O	2.20	0.41
2:B:331:PHE:N	2:B:332:PRO:CD	2.83	0.41
4:D:191:ASP:C	4:D:310:GLN:HE22	2.19	0.41
1:A:986:THR:OG1	1:A:1013:GLU:OE1	2.33	0.40
4:D:296:PRO:HG2	4:D:299:LEU:HD12	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	199/264 (75%)	190 (96%)	8 (4%)	1 (0%)	29	65
2	B	102/114 (90%)	94 (92%)	7 (7%)	1 (1%)	15	51
3	C	72/122 (59%)	67 (93%)	5 (7%)	0	100	100
4	D	154/251 (61%)	137 (89%)	16 (10%)	1 (1%)	25	62
All	All	527/751 (70%)	488 (93%)	36 (7%)	3 (1%)	25	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	337	LEU
4	D	277	GLY
1	A	884	PRO

### 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	180/232 (78%)	177 (98%)	3 (2%)	60	82
2	B	93/102 (91%)	93 (100%)	0	100	100
3	C	69/103 (67%)	69 (100%)	0	100	100
4	D	135/215 (63%)	134 (99%)	1 (1%)	84	93
All	All	477/652 (73%)	473 (99%)	4 (1%)	81	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	909	SER
1	A	956	LEU
1	A	975	THR
4	D	323	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	913	HIS
1	A	938	ASN
2	B	336	HIS
4	D	179	GLN
4	D	307	GLN
4	D	310	GLN
4	D	314	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](#)

3 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	0.63	0	17,19,21	1.99	4 (23%)
5	NAG	E	2	5	14,14,15	0.40	0	17,19,21	1.31	2 (11%)
5	BMA	E	3	5	11,11,12	0.56	0	15,15,17	2.84	8 (53%)

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	-	1/6/23/26	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

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	3	BMA	O2-C2-C3	-5.85	98.43	110.14
5	E	3	BMA	C2-C3-C4	4.60	118.85	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	3	BMA	O3-C3-C4	4.40	120.53	110.35
5	E	1	NAG	C2-N2-C7	4.38	129.14	122.90
5	E	1	NAG	C1-C2-N2	4.38	117.97	110.49
5	E	2	NAG	C1-O5-C5	3.61	117.08	112.19
5	E	3	BMA	C1-O5-C5	3.56	117.01	112.19
5	E	3	BMA	O3-C3-C2	3.51	116.71	109.99
5	E	2	NAG	C4-C3-C2	-2.91	106.76	111.02
5	E	3	BMA	O5-C5-C6	2.86	111.68	107.20
5	E	1	NAG	O5-C1-C2	-2.53	107.29	111.29
5	E	3	BMA	C6-C5-C4	-2.20	107.84	113.00
5	E	1	NAG	O7-C7-N2	2.20	126.00	121.95
5	E	3	BMA	C1-C2-C3	2.11	112.26	109.67

There are no chirality outliers.

All (1) torsion outliers are listed below:

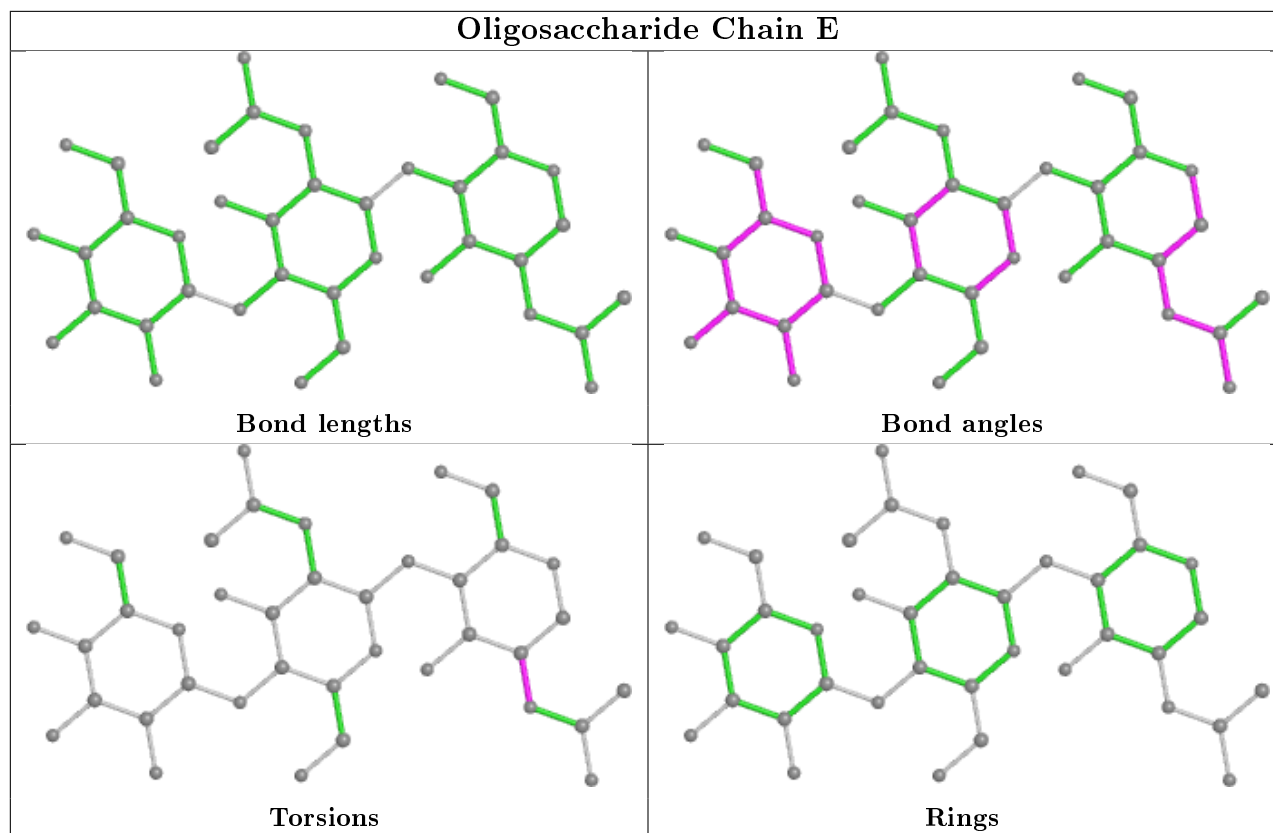
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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





## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
6	SRT	B	1399	-	3,9,9	0.96	0	6,12,12	0.79	0
6	SRT	B	1397	-	3,9,9	0.41	0	6,12,12	1.10	1 (16%)
7	ACT	B	1400	-	1,3,3	0.04	0	0,3,3	0.00	-
6	SRT	B	1398	-	3,9,9	0.94	0	6,12,12	0.51	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
6	SRT	B	1399	-	-	4/4/12/12	-
6	SRT	B	1397	-	-	0/4/12/12	-
6	SRT	B	1398	-	-	4/4/12/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1397	SRT	C4-C3-C2	-2.32	108.12	113.11

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1399	SRT	C1-C2-C3-C4
6	B	1399	SRT	O2-C2-C3-O3
6	B	1398	SRT	C1-C2-C3-O3
6	B	1398	SRT	C1-C2-C3-C4
6	B	1398	SRT	O2-C2-C3-O3
6	B	1399	SRT	C1-C2-C3-O3
6	B	1398	SRT	O2-C2-C3-C4
6	B	1399	SRT	O2-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	201/264 (76%)	0.46	4 (1%) 65 50	97, 131, 194, 234	0
2	B	104/114 (91%)	0.62	4 (3%) 40 25	88, 109, 185, 237	0
3	C	80/122 (65%)	0.47	3 (3%) 40 25	96, 151, 213, 234	0
4	D	156/251 (62%)	0.66	6 (3%) 40 25	86, 113, 186, 220	0
All	All	541/751 (72%)	0.55	17 (3%) 49 32	86, 125, 200, 237	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	81	PHE	4.1
2	B	334	ALA	3.9
3	C	137	ASP	3.2
4	D	299	LEU	2.5
2	B	333	LEU	2.5
4	D	303	TYR	2.3
4	D	300	ALA	2.3
2	B	356	ILE	2.2
2	B	331	PHE	2.2
1	A	1050	ILE	2.1
1	A	896	LEU	2.1
4	D	220	PHE	2.1
3	C	112	ILE	2.1
4	D	194	TYR	2.1
1	A	1059	TYR	2.1
4	D	309	LEU	2.0
1	A	1061	PHE	2.0

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

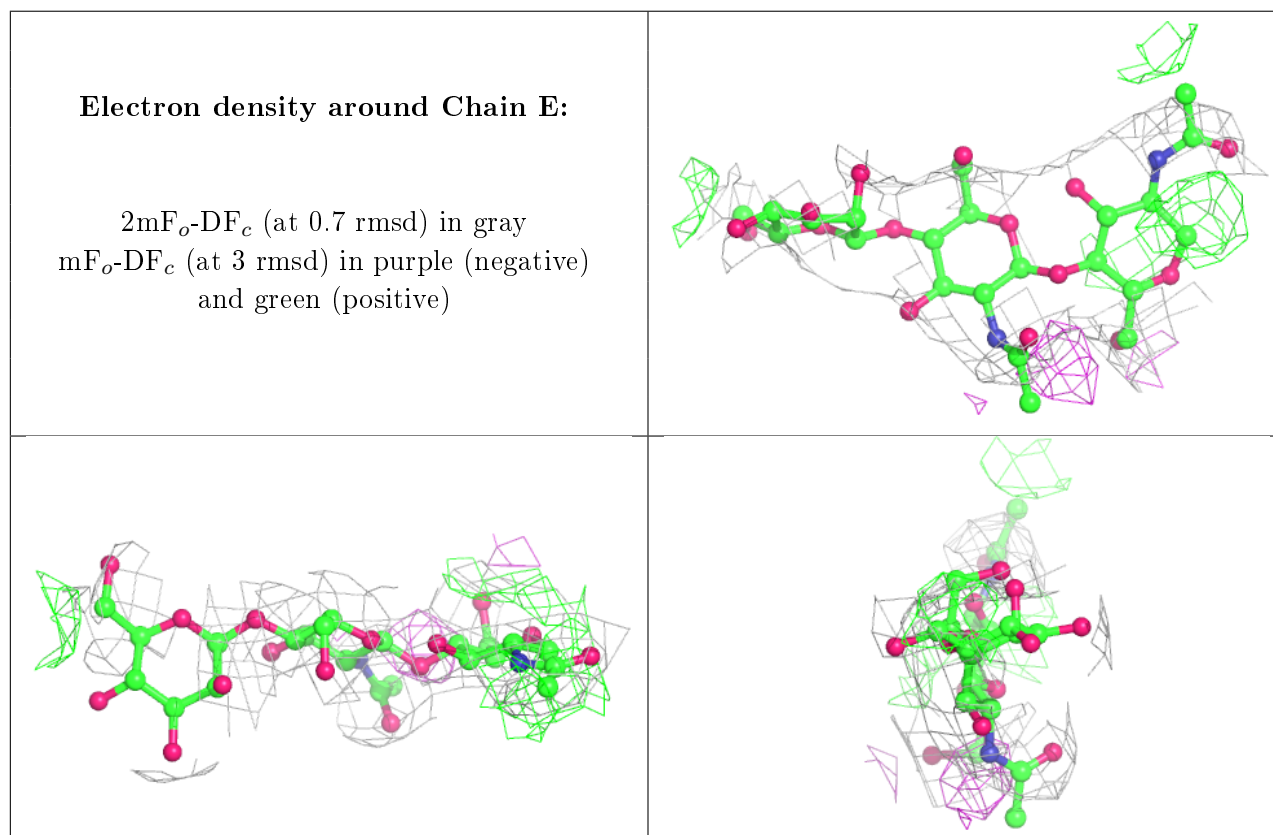
There are no non-standard protein/DNA/RNA residues in this entry.

### 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	BMA	E	3	11/12	0.53	0.19	204,224,237,238	0
5	NAG	E	1	14/15	0.90	0.20	130,157,168,180	0
5	NAG	E	2	14/15	0.90	0.21	148,184,204,216	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.



### 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SRT	B	1399	10/10	0.57	0.50	139,171,181,184	0
6	SRT	B	1397	10/10	0.65	0.27	130,167,173,175	0
6	SRT	B	1398	10/10	0.70	0.35	119,150,174,176	0
7	ACT	B	1400	4/4	0.88	0.41	94,106,107,108	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.