



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 03:34 am GMT

PDB ID : 6G3W
Title : Crystal structure of the BIR3 - SERK2 complex from Arabidopsis thaliana.
Authors : Hothorn, M.; Hohmann, U.
Deposited on : 2018-03-26
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

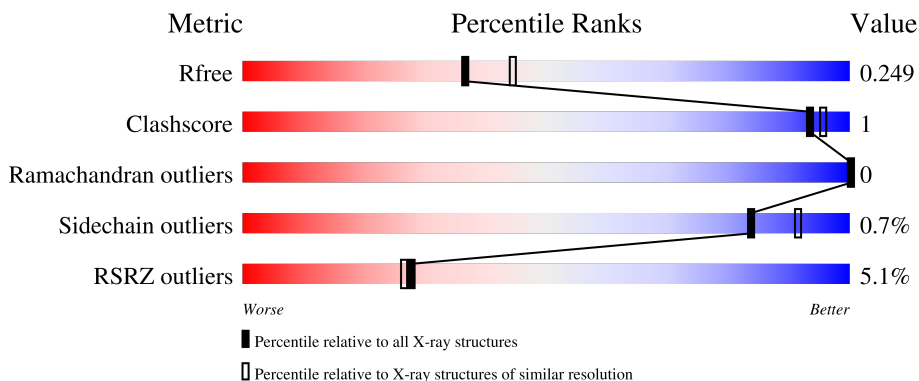
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 $\leq 5\%$. 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	217	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 14%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2% 80% 6% 15%</p>
1	C	217	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 16%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 83% • 15%</p>
2	B	196	<div style="display: flex; align-items: center;"> <div style="width: 1%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 93%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">% 94% • •</p>
2	D	196	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">12% 91% • • •</p>
3	E	3	<div style="display: flex; align-items: center;"> <div style="width: 33%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 33%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">33% 33% 33%</p>

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Mol	Chain	Length	Quality of chain
3	F	3	 67% 33%

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 5958 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 Somatic embryogenesis receptor kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	185	1411	890	239	275	7	0	0	0
1	C	184	1410	888	241	274	7	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	LEU	-	expression tag	UNP Q9XIC7
A	218	GLU	-	expression tag	UNP Q9XIC7
A	219	ASN	-	expression tag	UNP Q9XIC7
A	220	LEU	-	expression tag	UNP Q9XIC7
A	221	TYR	-	expression tag	UNP Q9XIC7
A	222	PHE	-	expression tag	UNP Q9XIC7
A	223	GLN	-	expression tag	UNP Q9XIC7
A	224	GLY	-	expression tag	UNP Q9XIC7
A	225	ALA	-	expression tag	UNP Q9XIC7
A	226	TRP	-	expression tag	UNP Q9XIC7
A	227	SER	-	expression tag	UNP Q9XIC7
A	228	HIS	-	expression tag	UNP Q9XIC7
A	229	PRO	-	expression tag	UNP Q9XIC7
A	230	GLN	-	expression tag	UNP Q9XIC7
A	231	PHE	-	expression tag	UNP Q9XIC7
A	232	GLU	-	expression tag	UNP Q9XIC7
A	233	LYS	-	expression tag	UNP Q9XIC7
A	234	GLY	-	expression tag	UNP Q9XIC7
A	235	SER	-	expression tag	UNP Q9XIC7
A	236	HIS	-	expression tag	UNP Q9XIC7
A	237	HIS	-	expression tag	UNP Q9XIC7
A	238	HIS	-	expression tag	UNP Q9XIC7
A	239	HIS	-	expression tag	UNP Q9XIC7
A	240	HIS	-	expression tag	UNP Q9XIC7
A	241	HIS	-	expression tag	UNP Q9XIC7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	242	HIS	-	expression tag	UNP Q9XIC7
A	243	HIS	-	expression tag	UNP Q9XIC7
A	244	HIS	-	expression tag	UNP Q9XIC7
C	217	LEU	-	expression tag	UNP Q9XIC7
C	218	GLU	-	expression tag	UNP Q9XIC7
C	219	ASN	-	expression tag	UNP Q9XIC7
C	220	LEU	-	expression tag	UNP Q9XIC7
C	221	TYR	-	expression tag	UNP Q9XIC7
C	222	PHE	-	expression tag	UNP Q9XIC7
C	223	GLN	-	expression tag	UNP Q9XIC7
C	224	GLY	-	expression tag	UNP Q9XIC7
C	225	ALA	-	expression tag	UNP Q9XIC7
C	226	TRP	-	expression tag	UNP Q9XIC7
C	227	SER	-	expression tag	UNP Q9XIC7
C	228	HIS	-	expression tag	UNP Q9XIC7
C	229	PRO	-	expression tag	UNP Q9XIC7
C	230	GLN	-	expression tag	UNP Q9XIC7
C	231	PHE	-	expression tag	UNP Q9XIC7
C	232	GLU	-	expression tag	UNP Q9XIC7
C	233	LYS	-	expression tag	UNP Q9XIC7
C	234	GLY	-	expression tag	UNP Q9XIC7
C	235	SER	-	expression tag	UNP Q9XIC7
C	236	HIS	-	expression tag	UNP Q9XIC7
C	237	HIS	-	expression tag	UNP Q9XIC7
C	238	HIS	-	expression tag	UNP Q9XIC7
C	239	HIS	-	expression tag	UNP Q9XIC7
C	240	HIS	-	expression tag	UNP Q9XIC7
C	241	HIS	-	expression tag	UNP Q9XIC7
C	242	HIS	-	expression tag	UNP Q9XIC7
C	243	HIS	-	expression tag	UNP Q9XIC7
C	244	HIS	-	expression tag	UNP Q9XIC7

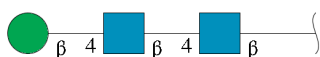
- Molecule 2 is a protein called Probable inactive receptor kinase At1g27190.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	189	1416	879	246	282	9	0	1	0
2	D	188	1402	869	245	279	9	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	215	GLU	-	expression tag	UNP O04567
B	216	ASN	-	expression tag	UNP O04567
B	217	LEU	-	expression tag	UNP O04567
B	218	TYR	-	expression tag	UNP O04567
B	219	PHE	-	expression tag	UNP O04567
B	220	GLN	-	expression tag	UNP O04567
D	215	GLU	-	expression tag	UNP O04567
D	216	ASN	-	expression tag	UNP O04567
D	217	LEU	-	expression tag	UNP O04567
D	218	TYR	-	expression tag	UNP O04567
D	219	PHE	-	expression tag	UNP O04567
D	220	GLN	-	expression tag	UNP O04567

- Molecule 3 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			
3	E	3	39	22	2	15	0	0	0
3	F	3	39	22	2	15	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



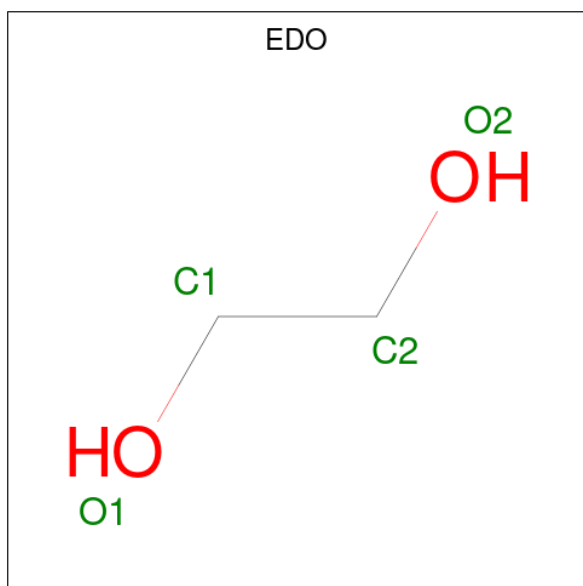
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total 14	8	1	5	0	0
4	B	1	Total 14	8	1	5	0	0
4	C	1	Total 14	8	1	5	0	0
4	C	1	Total 14	8	1	5	0	0
4	C	1	Total 14	8	1	5	0	0
4	D	1	Total 14	8	1	5	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

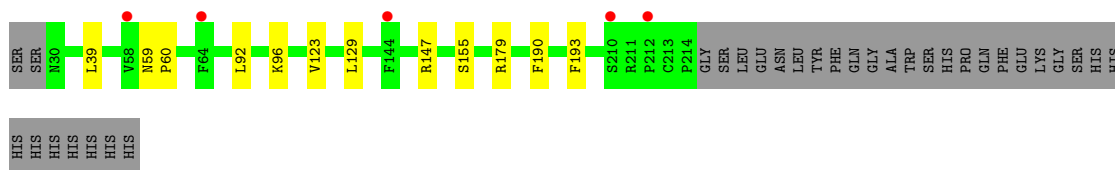
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	47	Total O 47 47	0	0
7	B	59	Total O 59 59	0	0
7	C	23	Total O 23 23	0	0
7	D	14	Total O 14 14	0	0

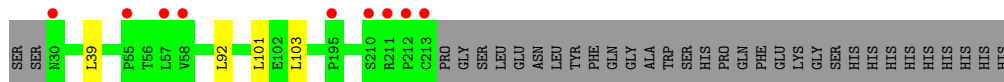
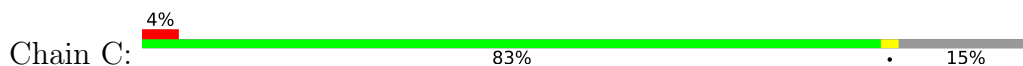
3 Residue-property plots [i](#)

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: Somatic embryogenesis receptor kinase 2



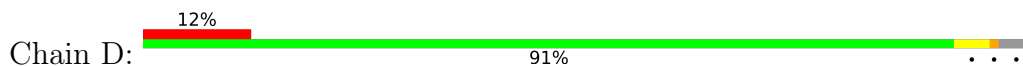
- Molecule 1: Somatic embryogenesis receptor kinase 2




- Molecule 2: Probable inactive receptor kinase At1g27190



- Molecule 2: Probable inactive receptor kinase At1g27190



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

Chain E:  33% 33% 33%



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

Chain F:  67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.18Å 52.16Å 308.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.41 – 2.20 49.41 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.41-2.20) 99.9 (49.41-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.217 , 0.248 0.221 , 0.249	Depositor DCC
R_{free} test set	2122 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtrriage
Anisotropy	0.424	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.035 for k,h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5958	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, PEG, NAG, EDO

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	0.54	0/1441	0.73	1/1975 (0.1%)
1	C	0.50	0/1439	0.65	0/1970
2	B	0.58	0/1438	0.71	0/1943
2	D	0.49	0/1421	0.67	0/1920
All	All	0.53	0/5739	0.69	1/7808 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ARG	NE-CZ-NH2	5.28	122.94	120.30

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	1411	0	1388	5	0
1	C	1410	0	1392	2	0
2	B	1416	0	1430	3	0
2	D	1402	0	1413	6	0
3	E	39	0	34	1	0
3	F	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	42	0	39	0	0
4	D	14	0	13	0	0
5	A	6	0	7	0	0
6	B	4	0	6	0	0
6	C	4	0	6	0	0
7	A	47	0	0	0	0
7	B	59	0	0	0	0
7	C	23	0	0	0	0
7	D	14	0	0	0	0
All	All	5958	0	5788	16	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 1.

All (16) 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:34:LEU:HD12	2:B:89:PRO:HG3	1.86	0.58
2:B:25:GLU:N	2:B:54:SER:HG	2.03	0.56
1:A:129:LEU:HD11	3:E:1:NAG:H82	1.87	0.55
2:B:34:LEU:HD12	2:B:89:PRO:CG	2.38	0.52
1:C:39:LEU:HD22	1:C:92:LEU:HD21	1.93	0.51
1:A:39:LEU:HD22	1:A:92:LEU:HD21	1.94	0.49
2:D:148:ASN:HD22	2:D:148:ASN:N	2.11	0.49
2:D:142:VAL:CG1	2:D:164:GLN:O	2.65	0.44
2:D:142:VAL:HG13	2:D:164:GLN:HB3	1.99	0.44
1:C:101:LEU:HD11	1:C:103:LEU:HD11	2.01	0.43
2:D:58:ILE:HD12	2:D:74:ILE:HD11	2.01	0.43
1:A:123:VAL:HB	1:A:147:ARG:HD2	2.02	0.42
2:D:48:TRP:HA	2:D:61:LEU:HD22	2.02	0.42
1:A:190:PHE:HA	1:A:193:PHE:CD2	2.56	0.40
1:A:59:ASN:HB2	1:A:60:PRO:HD2	2.03	0.40
2:D:35:LYS:NZ	2:D:45:LEU:O	2.53	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	183/217 (84%)	175 (96%)	8 (4%)	0	100	100
1	C	182/217 (84%)	174 (96%)	8 (4%)	0	100	100
2	B	188/196 (96%)	180 (96%)	8 (4%)	0	100	100
2	D	186/196 (95%)	177 (95%)	9 (5%)	0	100	100
All	All	739/826 (90%)	706 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	168/197 (85%)	166 (99%)	2 (1%)	71	83
1	C	168/197 (85%)	168 (100%)	0	100	100
2	B	167/173 (96%)	167 (100%)	0	100	100
2	D	165/173 (95%)	162 (98%)	3 (2%)	59	72
All	All	668/740 (90%)	663 (99%)	5 (1%)	84	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	A	155	SER

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Mol	Chain	Res	Type
2	D	142	VAL
2	D	148	ASN
2	D	188	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	99	GLN
1	C	30	ASN
1	C	81	ASN
2	D	148	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](#)

6 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	$\# Z > 2$
3	NAG	E	1	3,1	14,14,15	0.40	0	17,19,21	1.19	2 (11%)
3	NAG	E	2	3	14,14,15	0.53	0	17,19,21	1.25	3 (17%)
3	BMA	E	3	3	11,11,12	0.43	0	15,15,17	0.75	0
3	NAG	F	1	3,1	14,14,15	0.40	0	17,19,21	1.06	0
3	NAG	F	2	3	14,14,15	0.32	0	17,19,21	1.06	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	F	3	3	11,11,12	0.44	0	15,15,17	0.62	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
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	BMA	E	3	3	-	1/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	NAG	C1-O5-C5	2.75	115.92	112.19
3	E	1	NAG	O5-C1-C2	-2.41	107.48	111.29
3	F	2	NAG	C8-C7-N2	2.31	120.01	116.10
3	E	2	NAG	C2-N2-C7	2.28	126.15	122.90
3	E	2	NAG	C4-C3-C2	-2.21	107.77	111.02
3	E	2	NAG	O4-C4-C5	2.11	114.54	109.30
3	F	2	NAG	C2-N2-C7	2.02	125.78	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

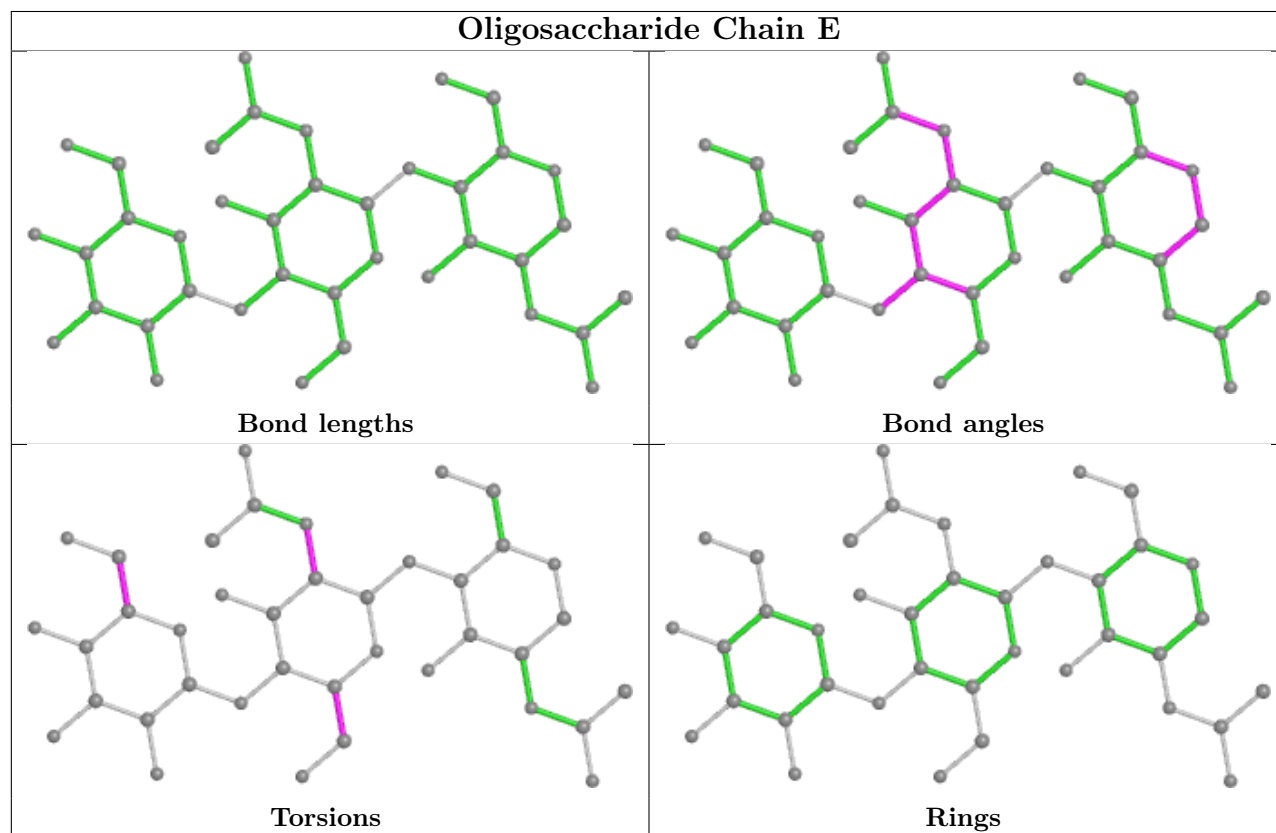
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C3-C2-N2-C7
3	E	3	BMA	C4-C5-C6-O6

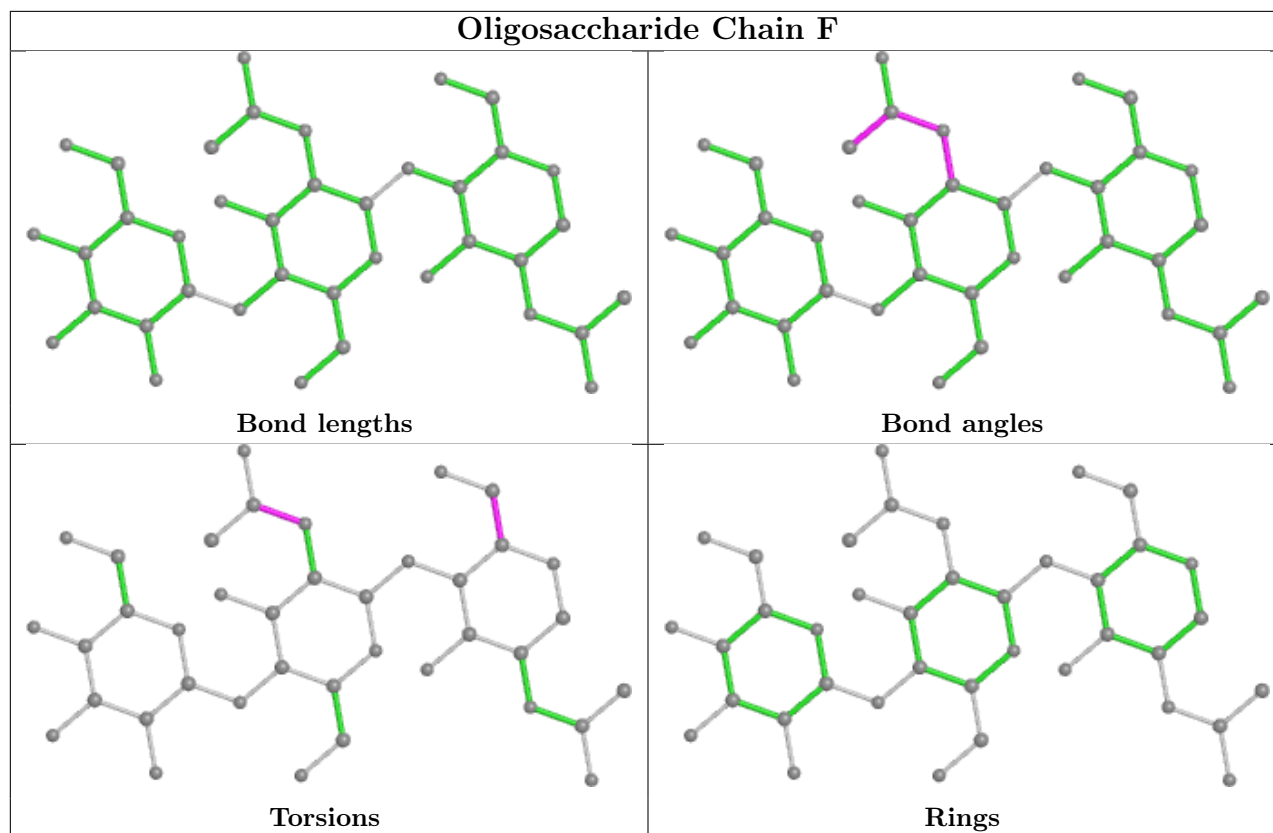
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	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.





5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
5	PEG	A	308	-	5,5,6	0.54	0	4,4,5	0.51	0
6	EDO	B	302	-	3,3,3	0.54	0	2,2,2	0.21	0
4	NAG	C	302	1	14,14,15	0.52	0	17,19,21	1.46	3 (17%)
4	NAG	C	301	1	14,14,15	0.35	0	17,19,21	0.76	0
4	NAG	B	301	2	14,14,15	0.57	0	17,19,21	0.92	0
6	EDO	C	304	-	3,3,3	0.57	0	2,2,2	0.13	0
4	NAG	C	303	1	14,14,15	0.45	0	17,19,21	1.29	1 (5%)
4	NAG	D	301	2	14,14,15	0.59	0	17,19,21	0.93	1 (5%)
4	NAG	A	301	1	14,14,15	0.34	0	17,19,21	0.73	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	PEG	A	308	-	-	1/3/3/4	-
6	EDO	B	302	-	-	0/1/1/1	-
4	NAG	C	302	1	-	1/6/23/26	0/1/1/1
4	NAG	C	301	1	-	0/6/23/26	0/1/1/1
4	NAG	B	301	2	-	0/6/23/26	0/1/1/1
6	EDO	C	304	-	-	0/1/1/1	-
4	NAG	C	303	1	-	0/6/23/26	0/1/1/1
4	NAG	D	301	2	-	0/6/23/26	0/1/1/1
4	NAG	A	301	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	303	NAG	C1-O5-C5	4.37	118.11	112.19
4	C	302	NAG	C1-O5-C5	3.34	116.72	112.19
4	C	302	NAG	O5-C5-C6	2.68	111.40	107.20
4	D	301	NAG	C1-O5-C5	2.63	115.76	112.19
4	C	302	NAG	C4-C3-C2	-2.23	107.75	111.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	302	NAG	O5-C5-C6-O6
5	A	308	PEG	O2-C3-C4-O4

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

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, 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	185/217 (85%)	-0.20	5 (2%) 54 52	33, 49, 77, 107	0
1	C	184/217 (84%)	0.11	9 (4%) 29 28	43, 64, 104, 121	0
2	B	189/196 (96%)	0.02	1 (0%) 91 90	34, 45, 73, 97	0
2	D	188/196 (95%)	0.66	23 (12%) 4 3	60, 79, 107, 125	0
All	All	746/826 (90%)	0.15	38 (5%) 28 26	33, 60, 98, 125	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	58	VAL	4.3
2	D	160	SER	3.4
2	D	176	LEU	3.1
1	A	58	VAL	3.1
2	D	210	ARG	3.1
1	A	64	PHE	3.1
2	D	54	SER	3.0
2	D	103	LEU	3.0
2	D	29	LEU	3.0
1	C	57	LEU	2.8
2	D	213	ALA	2.8
2	D	202	GLY	2.8
2	D	187	SER	2.8
2	D	205	GLY	2.7
1	C	30	ASN	2.7
2	D	159	GLY	2.7
1	C	55	PRO	2.6
2	D	212	GLY	2.6
2	D	101	LEU	2.6
1	A	210	SER	2.5
2	D	184	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	181	LEU	2.5
2	D	137	ILE	2.4
2	D	94	LEU	2.4
1	A	212	PRO	2.4
1	C	212	PRO	2.4
1	A	144	PHE	2.3
1	C	195	PRO	2.3
2	D	37	SER	2.3
2	D	188	GLU	2.3
2	D	143	GLU	2.2
2	D	133	LEU	2.2
1	C	210	SER	2.2
2	B	77	LEU	2.1
2	D	169	ASP	2.1
1	C	211	ARG	2.1
2	D	118	SER	2.1
1	C	213	CYS	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](#)

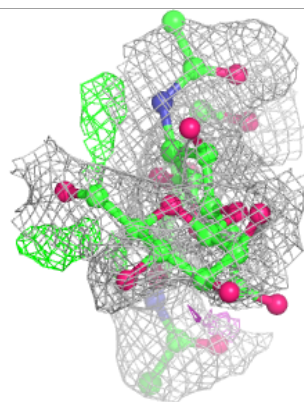
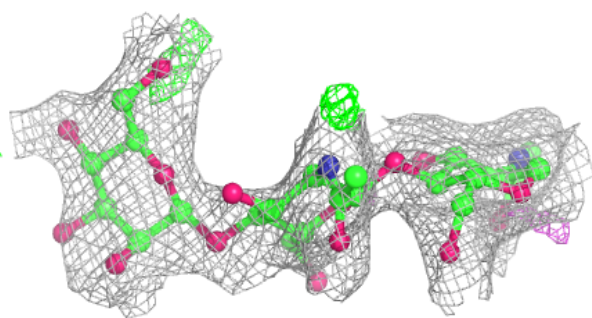
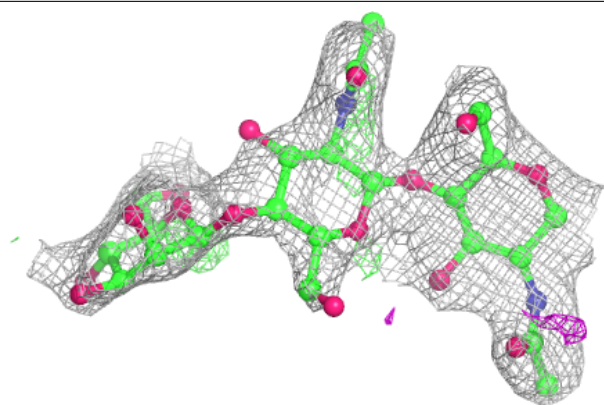
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	E	3	11/12	0.56	0.21	90,97,100,101	0
3	NAG	E	2	14/15	0.69	0.21	84,92,98,98	0
3	BMA	F	3	11/12	0.69	0.34	99,105,108,109	0
3	NAG	E	1	14/15	0.79	0.16	55,62,72,87	0
3	NAG	F	2	14/15	0.81	0.16	90,93,97,104	0
3	NAG	F	1	14/15	0.84	0.13	62,72,80,86	0

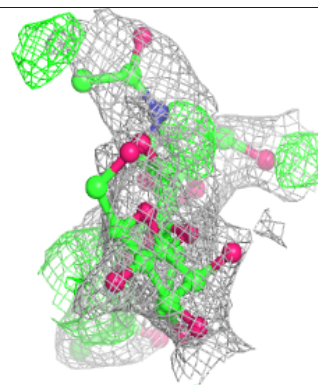
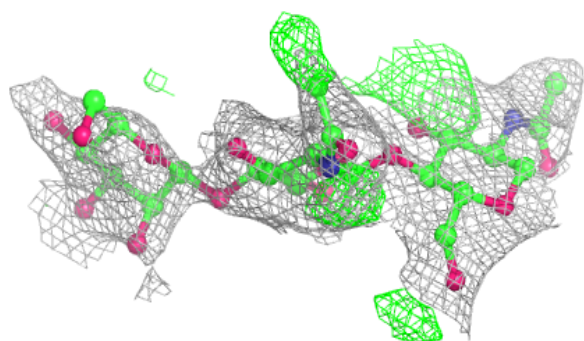
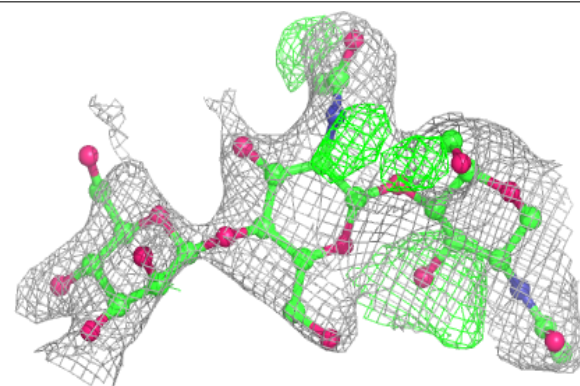
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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
4	NAG	D	301	14/15	0.46	0.24	91,94,98,98	0
6	EDO	C	304	4/4	0.74	0.35	66,66,66,69	0
5	PEG	A	308	6/7	0.79	0.24	64,65,74,74	0
4	NAG	C	301	14/15	0.81	0.18	155,164,180,180	0
4	NAG	C	303	14/15	0.85	0.14	66,76,79,81	0
4	NAG	A	301	14/15	0.86	0.16	71,81,86,87	0
4	NAG	C	302	14/15	0.86	0.13	63,72,86,91	0
4	NAG	B	301	14/15	0.88	0.10	64,71,80,82	0
6	EDO	B	302	4/4	0.96	0.12	55,58,58,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.