



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 10, 2023 – 06:40 PM EDT

PDB ID : 4JBS
Title : Crystal structure of the human Endoplasmic Reticulum Aminopeptidase 2 in complex with PHOSPHINIC PSEUDOTRIPEPTIDE inhibitor.
Authors : Saridakis, E.; Birtley, J.; Stratikos, E.; Mavridis, I.M.
Deposited on : 2013-02-20
Resolution : 2.79 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 ⓘ 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 : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

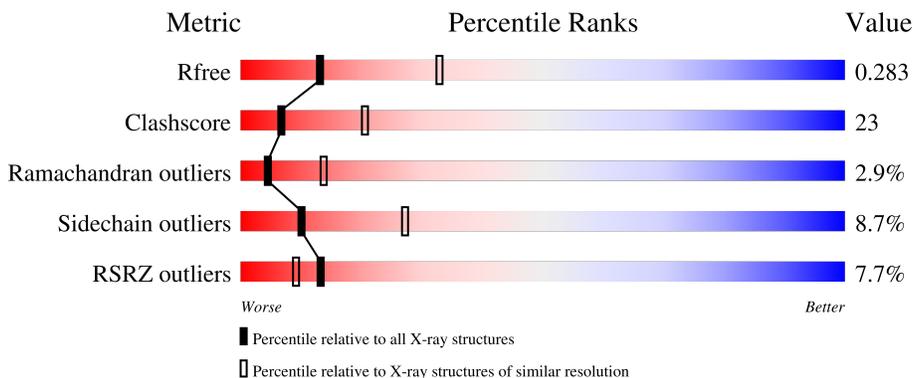
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	967	
1	B	967	
2	C	2	
2	D	2	
2	F	2	

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Mol	Chain	Length	Quality of chain
3	E	4	 25% 75%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14457 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 Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	869	7045	4547	1170	1301	27	2	2	0
1	B	854	6831	4416	1130	1259	26	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP Q6P179
A	2	VAL	-	cloning artifact	UNP Q6P179
A	961	ARG	-	expression tag	UNP Q6P179
A	962	HIS	-	expression tag	UNP Q6P179
A	963	HIS	-	expression tag	UNP Q6P179
A	964	HIS	-	expression tag	UNP Q6P179
A	965	HIS	-	expression tag	UNP Q6P179
A	966	HIS	-	expression tag	UNP Q6P179
A	967	HIS	-	expression tag	UNP Q6P179
B	1	MET	-	cloning artifact	UNP Q6P179
B	2	VAL	-	cloning artifact	UNP Q6P179
B	961	ARG	-	expression tag	UNP Q6P179
B	962	HIS	-	expression tag	UNP Q6P179
B	963	HIS	-	expression tag	UNP Q6P179
B	964	HIS	-	expression tag	UNP Q6P179
B	965	HIS	-	expression tag	UNP Q6P179
B	966	HIS	-	expression tag	UNP Q6P179
B	967	HIS	-	expression tag	UNP Q6P179

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



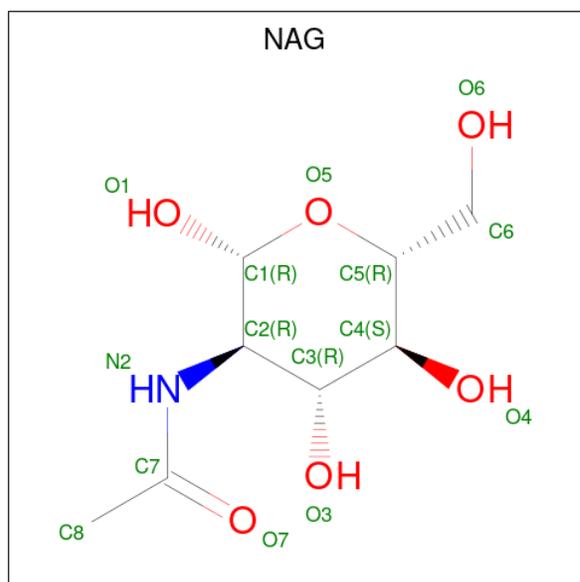
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0
2	F	2	28	16	2	10	0	0	0

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-alpha-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	4	50	28	2	20	0	0	0

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

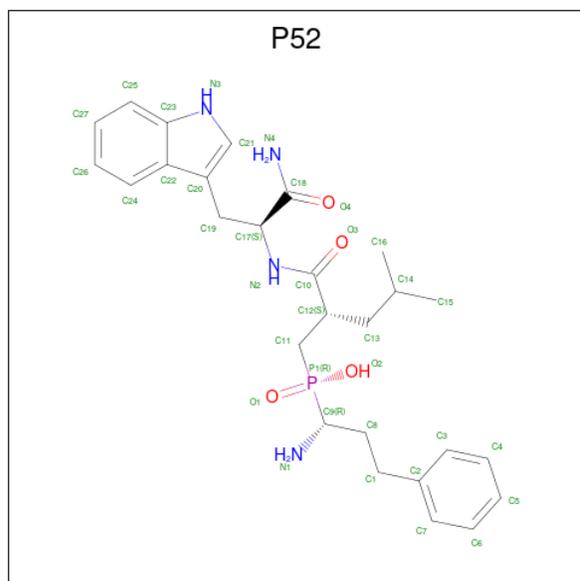


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

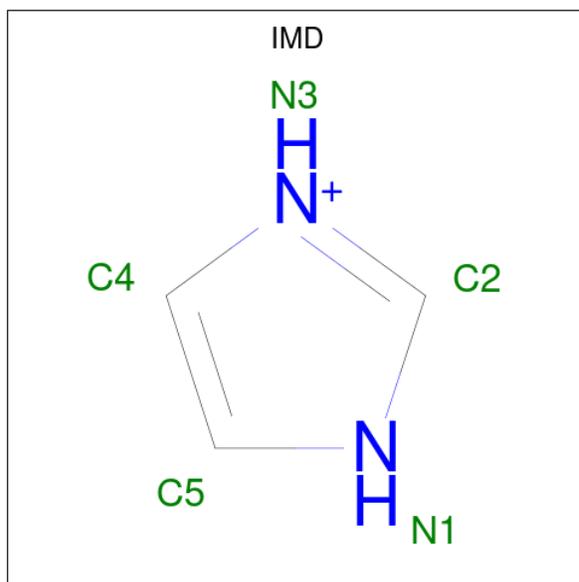
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

- Molecule 6 is Nalpha-[(2S)-2-{[(1R)-1-amino-3-phenylpropyl](hydroxy)phosphoryl]methyl}-4-methylpentanoyl]-L-tryptophanamide (three-letter code: P52) (formula: C₂₇H₃₇N₄O₄P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	1	0
			36	27	4	4	1		
6	B	1	Total	C	N	O	P	1	0
			36	27	4	4	1		

- Molecule 7 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N 5 3 2	0	0
7	A	1	Total C N 5 3 2	0	0

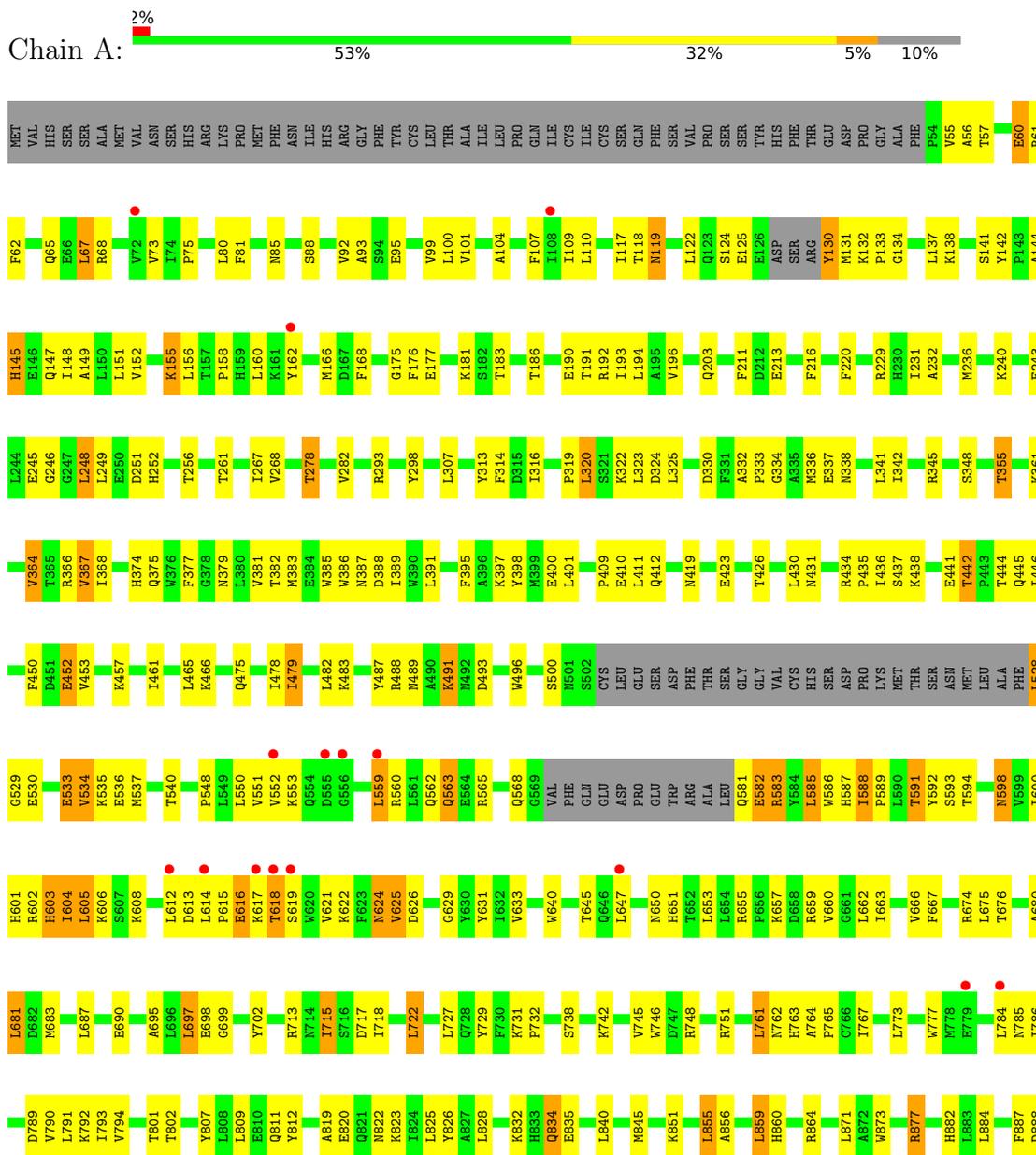
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	207	Total O 207 207	0	0
8	B	86	Total O 86 86	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: Endoplasmic reticulum aminopeptidase 2





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

Chain C: 100%



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

Chain D: 50%



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

Chain F: 50%



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

Chain E: 75%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.15Å 134.77Å 128.73Å 90.00° 90.28° 90.00°	Depositor
Resolution (Å)	10.99 – 2.79 48.77 – 2.79	Depositor EDS
% Data completeness (in resolution range)	94.7 (10.99-2.79) 99.8 (48.77-2.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.77Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.206 , 0.278 0.214 , 0.283	Depositor DCC
R_{free} test set	3225 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtrriage
Anisotropy	0.141	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.015 for -h,-l,-k 0.006 for -h,l,k 0.025 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14457	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, ZN, P52, IMD

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	0.27	0/7222	0.46	0/9787
1	B	0.26	0/6995	0.45	0/9488
All	All	0.27	0/14217	0.46	0/19275

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7045	0	6981	282	0
1	B	6831	0	6698	374	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	F	28	0	25	3	0
3	E	50	0	43	4	0
4	A	42	0	39	0	0
4	B	28	0	26	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	36	0	36	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	36	0	35	2	0
7	A	10	0	10	0	0
8	A	207	0	0	6	0
8	B	86	0	0	0	0
All	All	14457	0	13943	658	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 23.

The worst 5 of 658 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:A:56:ALA:HB1	1:A:57:THR:HA	1.31	1.09
1:B:374:HIS:HE1	1:B:392:LYS:HG2	1.29	0.96
1:B:565:ARG:HD2	1:B:584:TYR:HE2	1.28	0.94
1:B:582:GLU:N	1:B:583:ARG:HB2	1.85	0.92
1:B:104:ALA:HB2	1:B:158:PRO:HD3	1.50	0.91

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	863/967 (89%)	771 (89%)	76 (9%)	16 (2%)	8	23
1	B	842/967 (87%)	701 (83%)	107 (13%)	34 (4%)	3	8
All	All	1705/1934 (88%)	1472 (86%)	183 (11%)	50 (3%)	4	14

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	583	ARG
1	A	616	GLU
1	A	617	LYS
1	A	922	GLU

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	772/870 (89%)	699 (90%)	73 (10%)	8 23
1	B	733/870 (84%)	675 (92%)	58 (8%)	12 31
All	All	1505/1740 (86%)	1374 (91%)	131 (9%)	10 27

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	674	ARG
1	B	697	LEU
1	B	952	LEU
1	A	645	THR
1	A	625	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	624	ASN
1	B	833	HIS
1	B	651	HIS
1	B	763	HIS
1	B	870	GLN

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](#)

10 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
2	NAG	C	1	2,1	14,14,15	0.58	0	17,19,21	0.89	1 (5%)
2	NAG	C	2	2	14,14,15	0.48	0	17,19,21	0.96	1 (5%)
2	NAG	D	1	2,1	14,14,15	0.57	0	17,19,21	0.85	0
2	NAG	D	2	2	14,14,15	0.52	0	17,19,21	0.95	2 (11%)
3	NAG	E	1	1,3	14,14,15	0.49	0	17,19,21	1.95	3 (17%)
3	NAG	E	2	3	14,14,15	0.55	0	17,19,21	1.43	1 (5%)
3	MAN	E	3	3	11,11,12	0.59	0	15,15,17	2.02	4 (26%)
3	MAN	E	4	3	11,11,12	0.53	0	15,15,17	2.01	3 (20%)
2	NAG	F	1	2,1	14,14,15	0.54	0	17,19,21	0.74	0
2	NAG	F	2	2	14,14,15	0.59	0	17,19,21	1.08	1 (5%)

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	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	MAN	E	3	3	-	2/2/19/22	0/1/1/1

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

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4	MAN	C1-O5-C5	6.30	120.72	112.19
3	E	1	NAG	C1-O5-C5	5.18	119.21	112.19
3	E	2	NAG	C1-O5-C5	4.62	118.45	112.19
3	E	3	MAN	C2-C3-C4	4.34	118.41	110.89
3	E	1	NAG	C4-C3-C2	-4.00	105.16	111.02

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

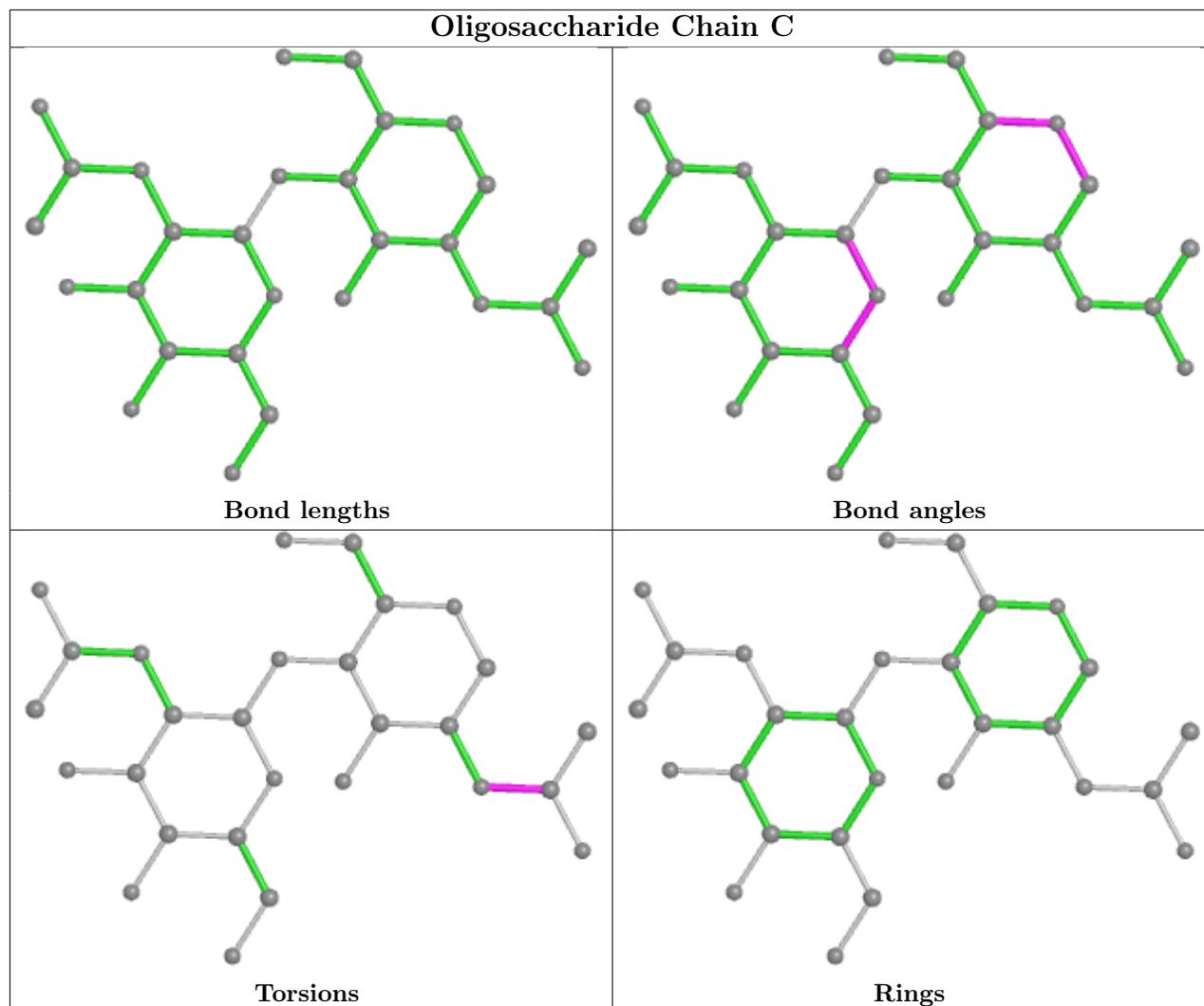
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C1-C2-N2-C7
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6

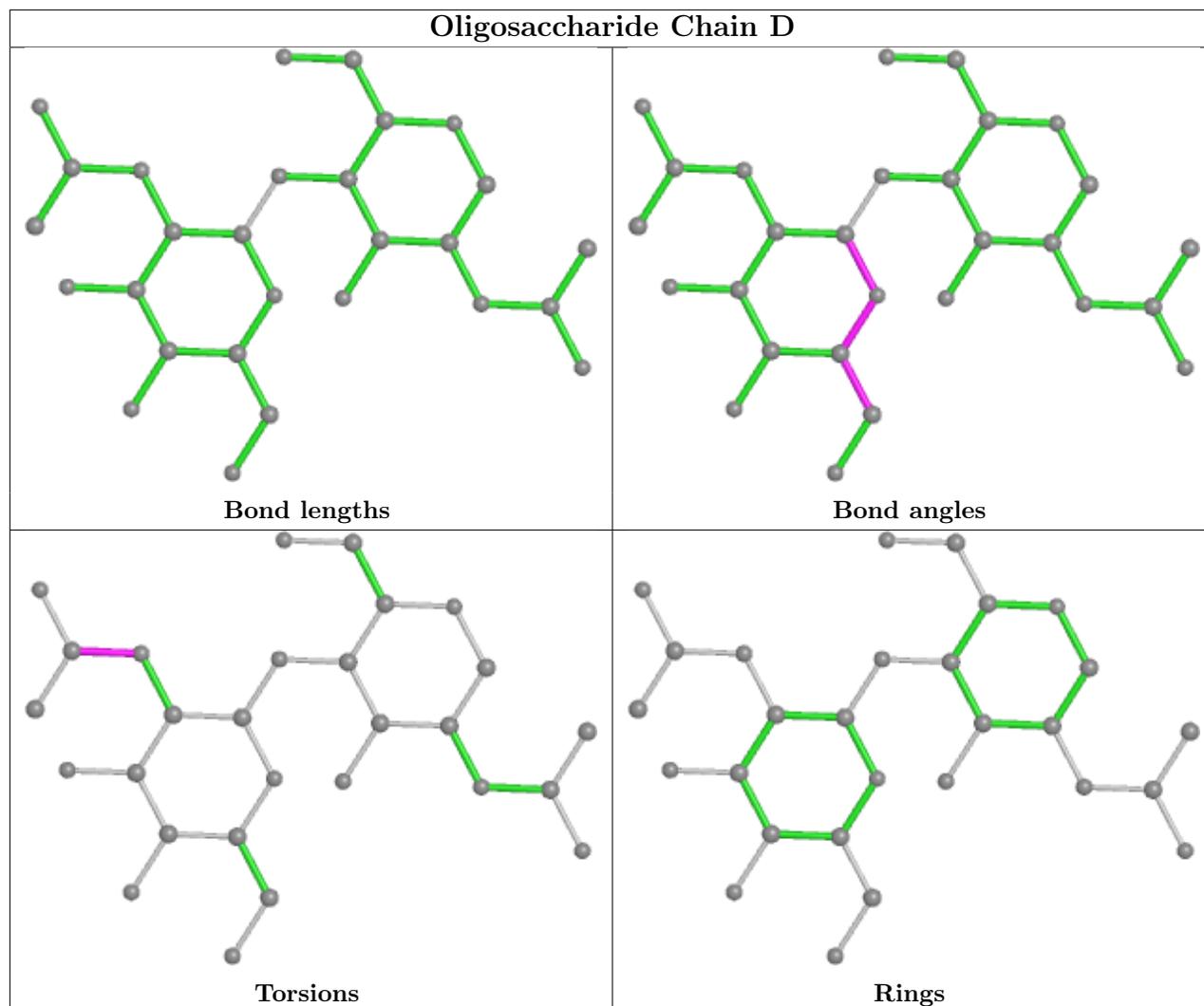
There are no ring outliers.

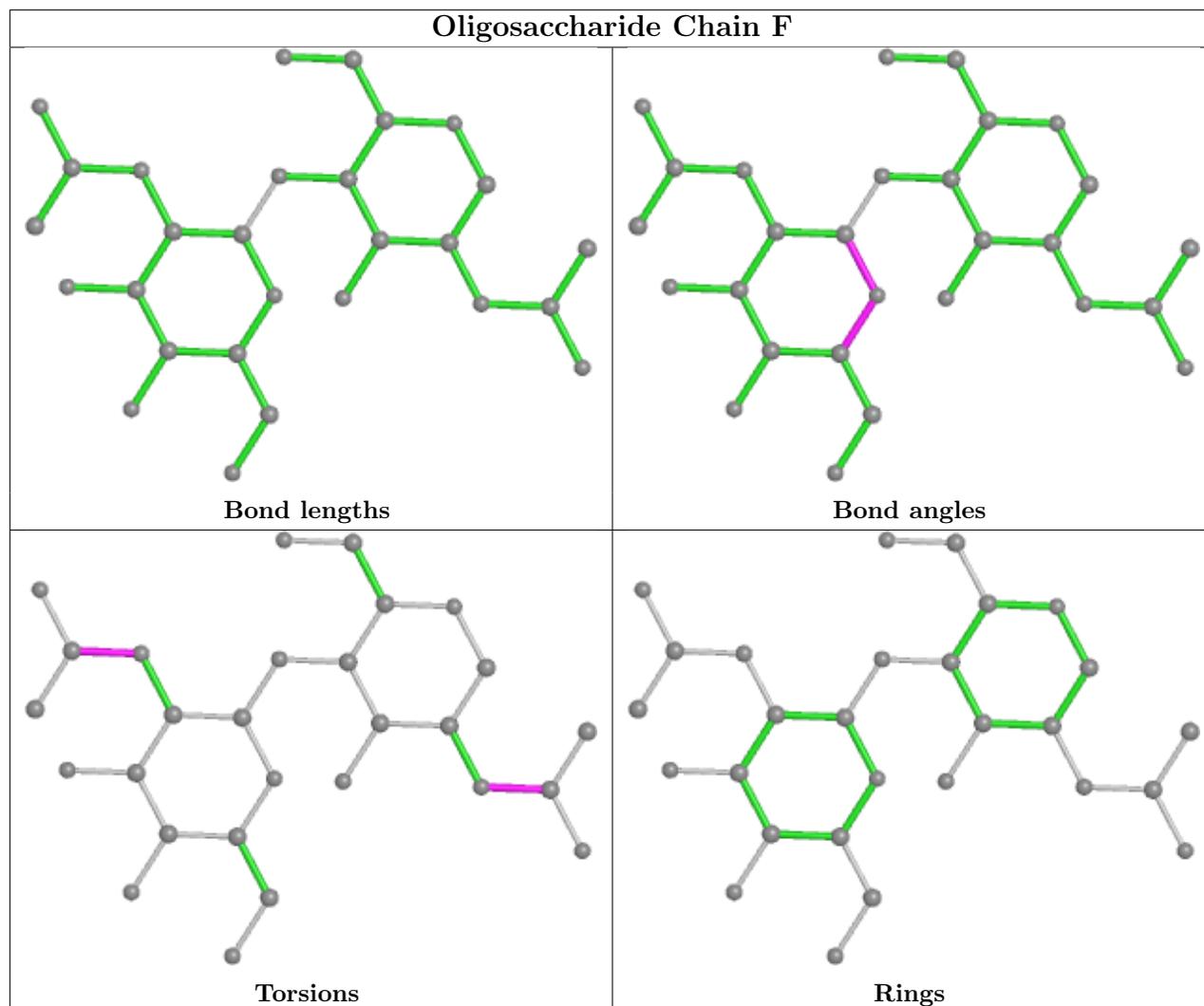
5 monomers are involved in 7 short contacts:

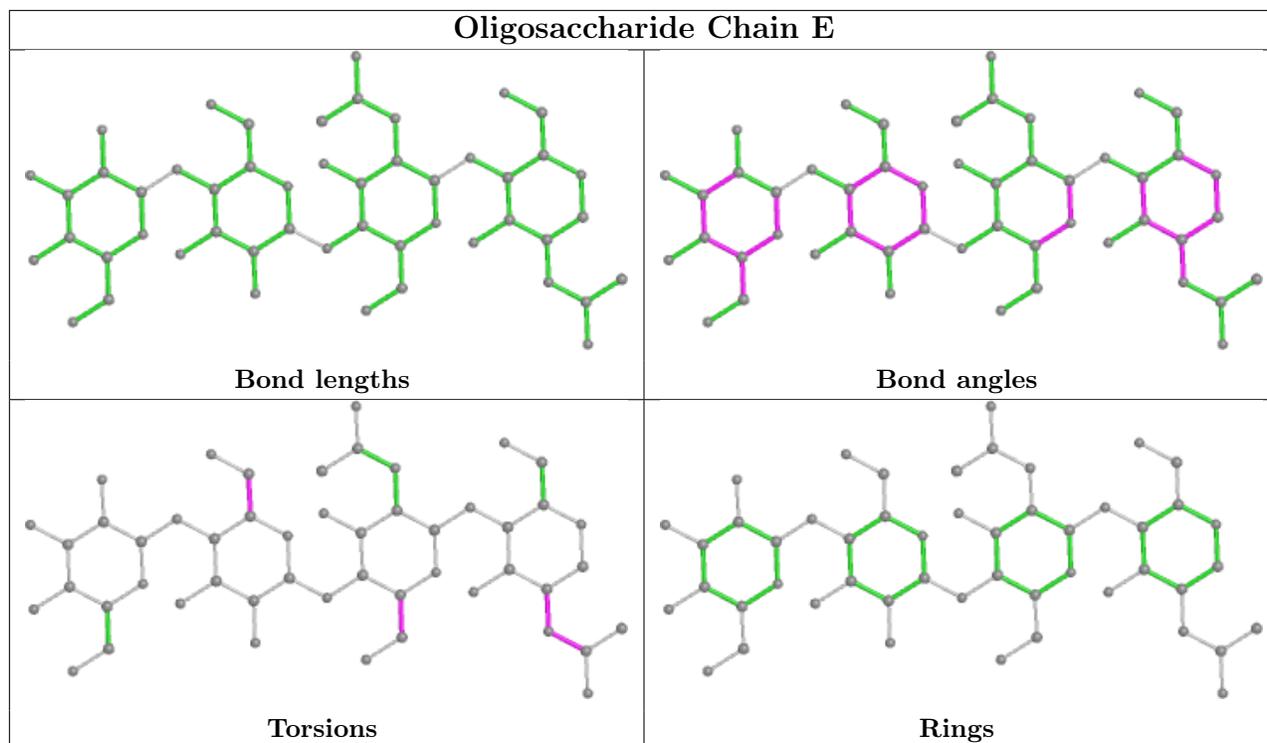
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	3	MAN	3	0
3	E	1	NAG	1	0
3	E	4	MAN	2	0
2	F	1	NAG	3	0
2	F	2	NAG	1	0

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](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	IMD	A	1011	-	3,5,5	0.38	0	4,5,5	0.49	0
4	NAG	A	1007	1	14,14,15	0.48	0	17,19,21	0.97	1 (5%)
6	P52	B	1010	5	33,38,38	3.83	5 (15%)	38,53,53	2.93	5 (13%)
7	IMD	A	1010	-	3,5,5	0.36	0	4,5,5	0.65	0
6	P52	A	1009	5	33,38,38	3.84	5 (15%)	38,53,53	2.27	5 (13%)
4	NAG	A	1005	1	14,14,15	0.49	0	17,19,21	0.97	1 (5%)
4	NAG	B	1007	1	14,14,15	0.57	0	17,19,21	1.23	1 (5%)
4	NAG	A	1006	1	14,14,15	0.77	0	17,19,21	0.90	0
4	NAG	B	1008	1	14,14,15	0.48	0	17,19,21	0.79	1 (5%)

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	IMD	A	1011	-	-	-	0/1/1/1
4	NAG	A	1007	1	-	4/6/23/26	0/1/1/1
6	P52	B	1010	5	-	14/29/36/36	0/3/3/3
7	IMD	A	1010	-	-	-	0/1/1/1
6	P52	A	1009	5	-	11/29/36/36	0/3/3/3
4	NAG	A	1005	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1007	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1006	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1008	1	-	2/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1009	P52	P1-C11	-19.75	1.60	1.79
6	B	1010	P52	P1-C11	-19.67	1.60	1.79
6	B	1010	P52	C9-N1	-6.77	1.29	1.48
6	A	1009	P52	C9-N1	-6.72	1.29	1.48
6	B	1010	P52	C18-N4	4.40	1.44	1.32

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1010	P52	C17-N2-C10	16.40	156.83	121.67
6	A	1009	P52	C17-N2-C10	11.86	147.10	121.67
4	B	1007	NAG	O5-C1-C2	3.55	116.89	111.29
4	A	1005	NAG	C1-O5-C5	2.87	116.08	112.19
6	A	1009	P52	O3-C10-N2	-2.65	118.02	122.93

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1007	NAG	C8-C7-N2-C2
4	A	1007	NAG	O7-C7-N2-C2
4	B	1007	NAG	C8-C7-N2-C2
4	B	1007	NAG	O7-C7-N2-C2

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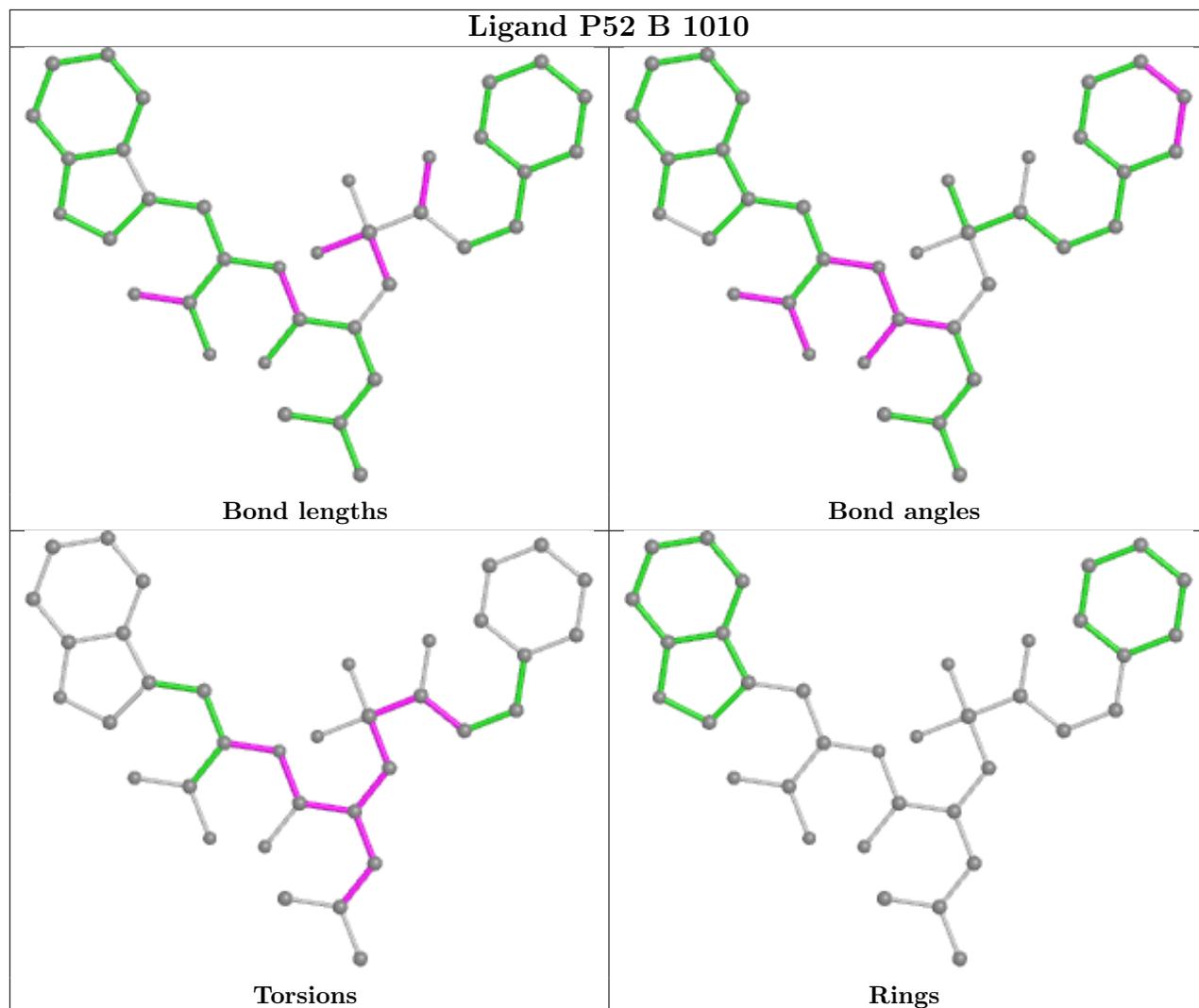
Mol	Chain	Res	Type	Atoms
4	B	1008	NAG	O7-C7-N2-C2

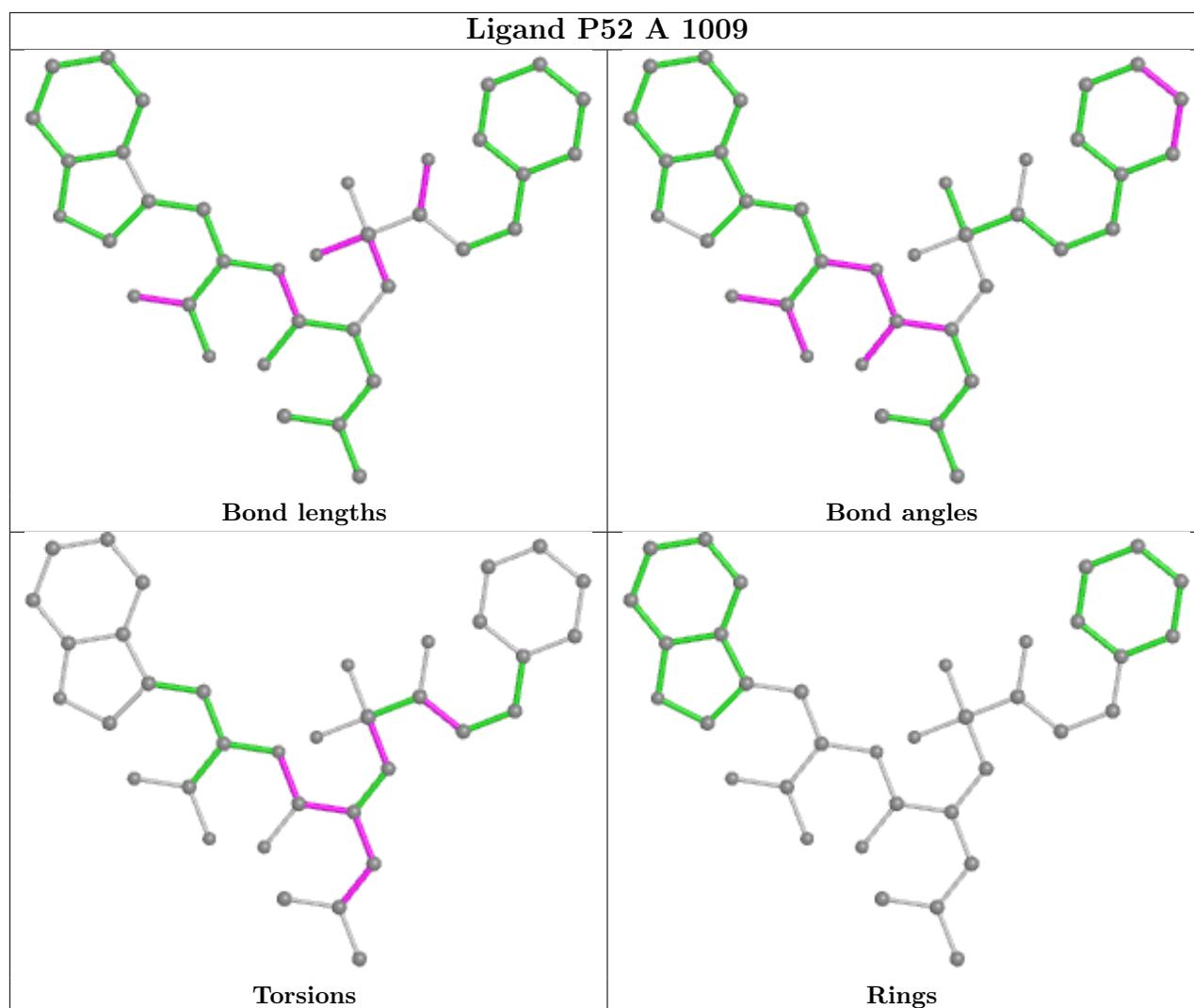
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1010	P52	2	0
6	A	1009	P52	3	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 than 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.





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	869/967 (89%)	-0.01	15 (1%) 70 67	21, 48, 86, 115	2 (0%)
1	B	854/967 (88%)	0.76	117 (13%) 3 2	29, 84, 120, 144	0
All	All	1723/1934 (89%)	0.37	132 (7%) 13 9	21, 62, 112, 144	2 (0%)

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	640	TRP	12.1
1	B	570	VAL	8.9
1	B	559	LEU	8.4
1	B	687	LEU	7.4
1	B	603	HIS	6.6

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.

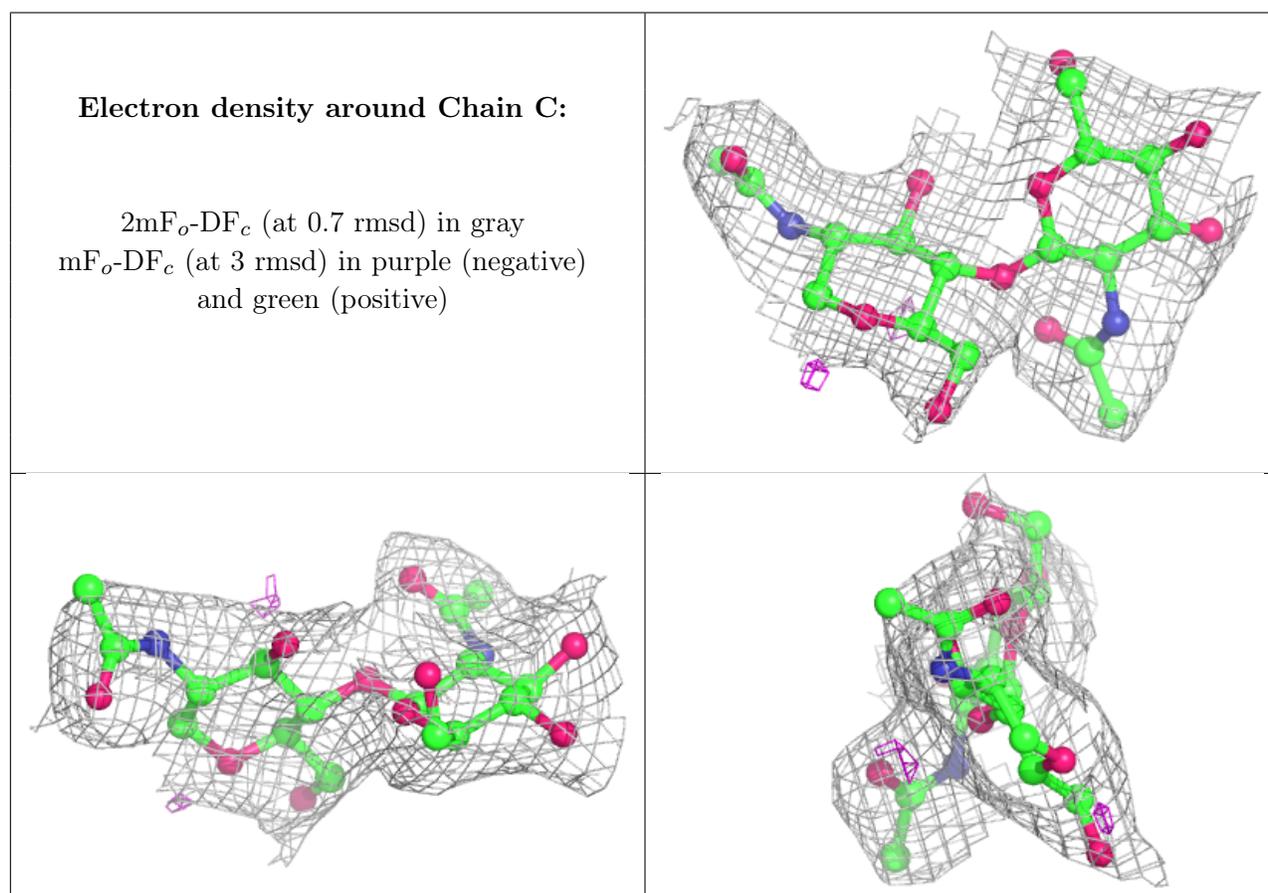
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MAN	E	4	11/12	0.70	0.33	91,109,129,132	0
3	MAN	E	3	11/12	0.83	0.17	70,86,98,107	0
2	NAG	F	2	14/15	0.86	0.20	62,94,102,102	0
2	NAG	C	2	14/15	0.88	0.21	62,80,91,93	0
3	NAG	E	2	14/15	0.90	0.16	48,71,91,97	0

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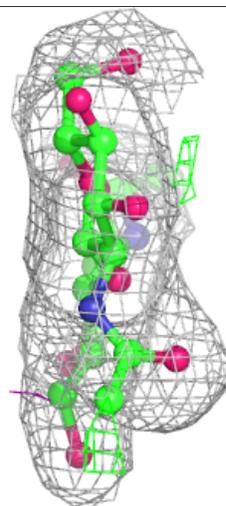
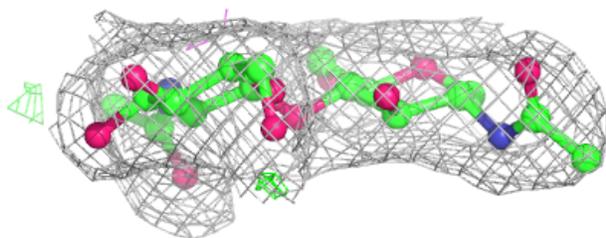
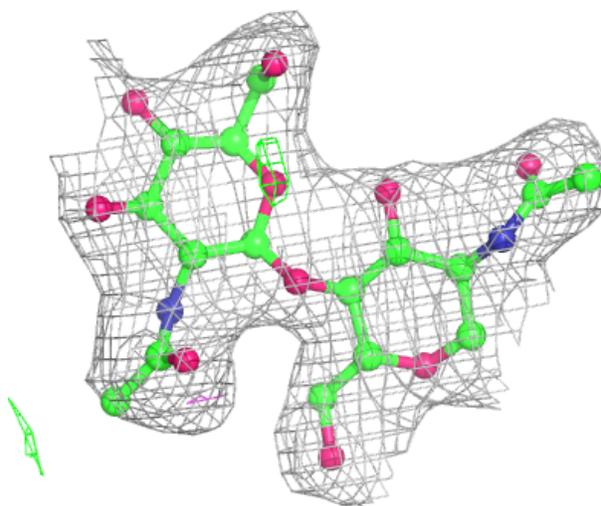
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	F	1	14/15	0.91	0.16	67,85,101,103	0
3	NAG	E	1	14/15	0.94	0.14	36,53,63,63	0
2	NAG	D	2	14/15	0.94	0.14	50,63,70,72	0
2	NAG	C	1	14/15	0.95	0.19	39,61,68,68	0
2	NAG	D	1	14/15	0.97	0.14	40,47,62,64	0

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.



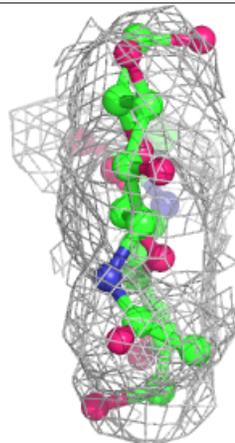
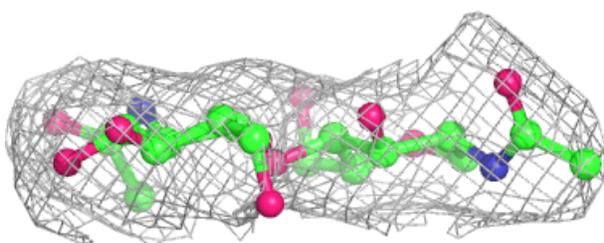
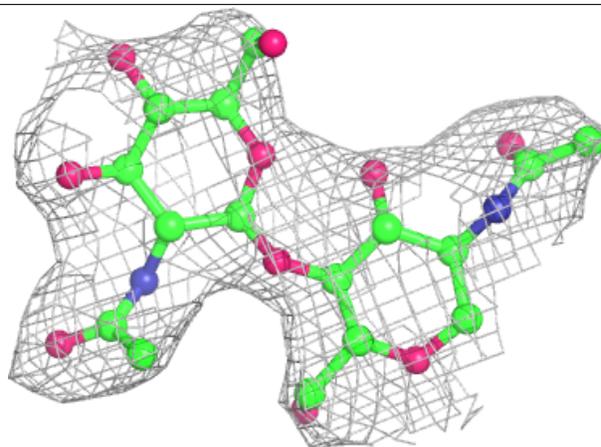
Electron density around Chain D:

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

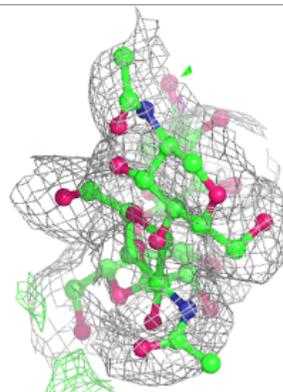
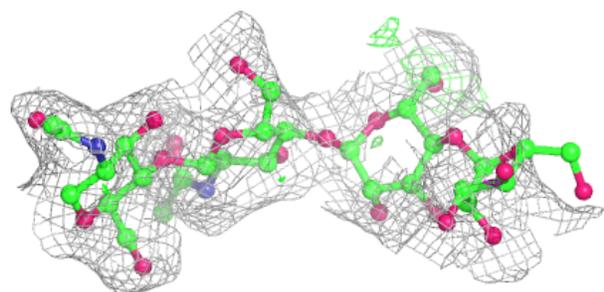
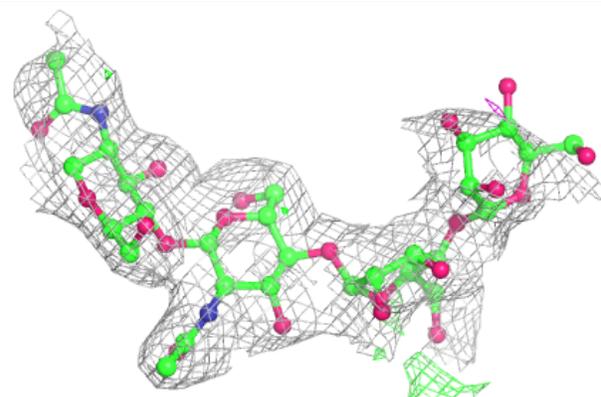


Electron density around Chain F:

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

**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)



6.4 Ligands

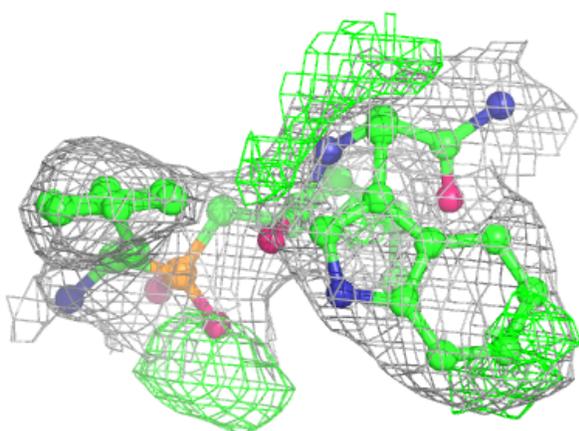
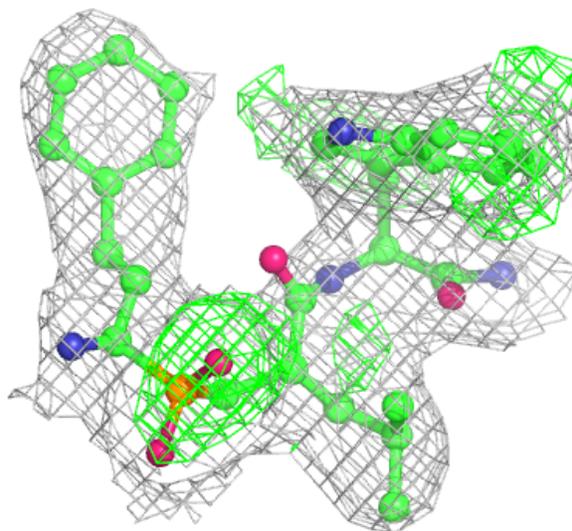
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

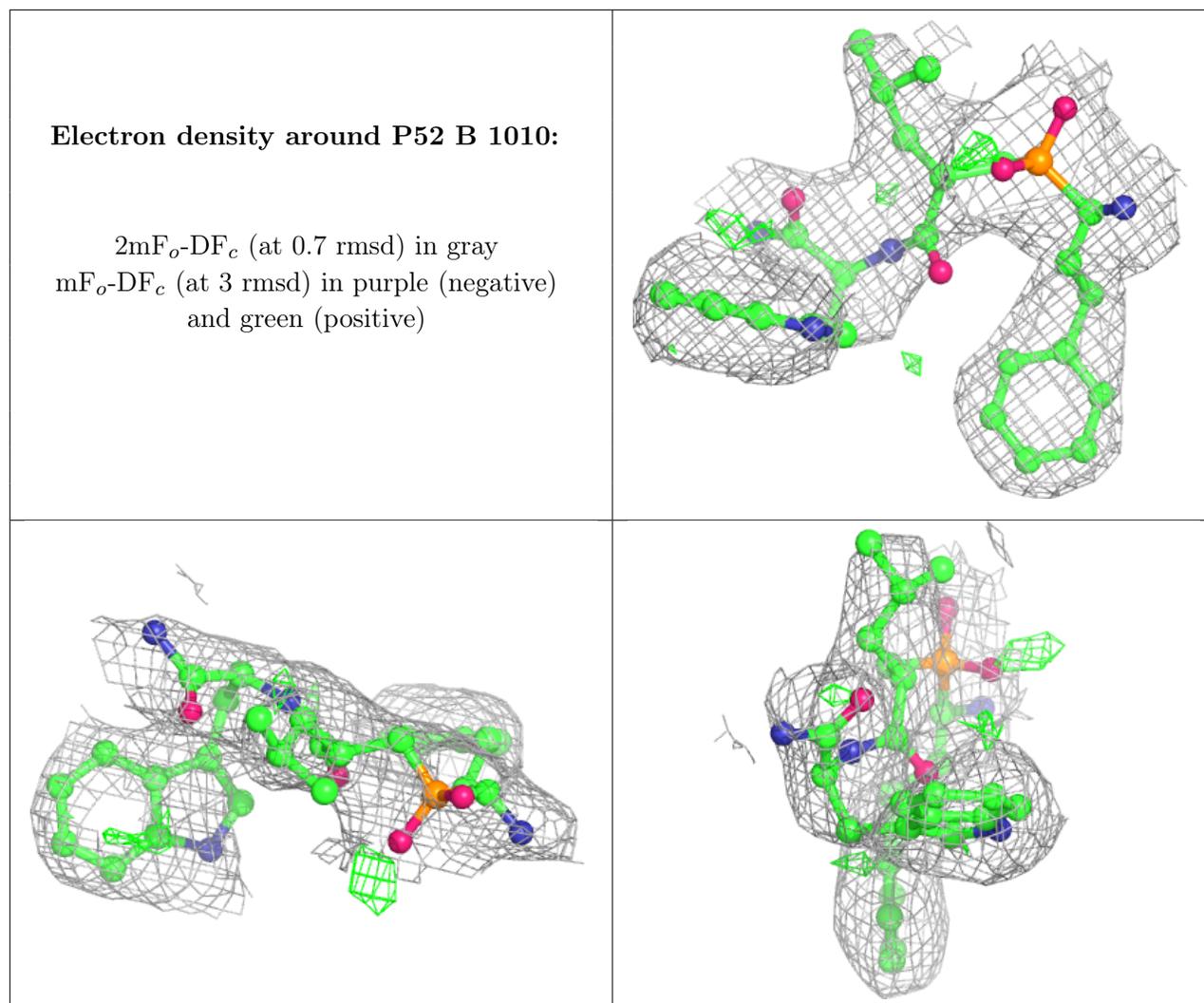
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	B	1007	14/15	0.77	0.27	85,112,123,137	0
7	IMD	A	1010	5/5	0.79	0.24	64,68,69,80	0
4	NAG	B	1008	14/15	0.83	0.29	79,109,118,122	0
4	NAG	A	1007	14/15	0.85	0.18	80,105,111,113	0
4	NAG	A	1006	14/15	0.88	0.26	76,88,106,106	0
7	IMD	A	1011	5/5	0.91	0.22	57,60,69,70	0
4	NAG	A	1005	14/15	0.94	0.17	65,78,82,84	0
6	P52	A	1009	36/36	0.95	0.31	25,38,60,66	3
6	P52	B	1010	36/36	0.95	0.32	33,57,88,90	4
5	ZN	B	1009	1/1	0.98	0.23	47,47,47,47	0
5	ZN	A	1008	1/1	0.99	0.22	25,25,25,25	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 P52 A 1009:

$2mF_o-DF_c$ (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.