WORLDWIDE wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Dec 12, 2023 – 11:53 pm GMT

PDB ID	:	4BWL
Title	:	Structure of the Y137A mutant of E. coli N-acetylneuraminic acid lyase in complex with pyruvate, N-acetyl-D-mannosamine and N- acetylneuraminic acid
Authors	:	Campeotto, I.; Phillips, S.E.V.; Pearson, A.R.; Nelson, A.; Berry, A.
Deposited on	:	2013-07-03
Resolution	:	2.00 Å(reported)

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

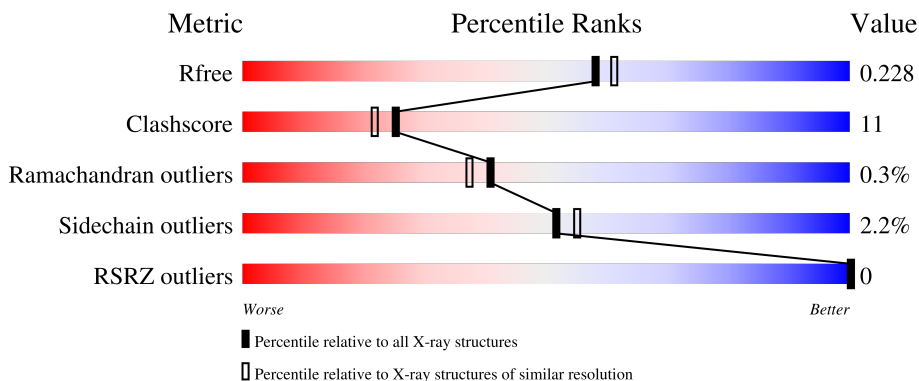|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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	Percentile Ranks	Value
Rfree		0.228
Clashscore		11
Ramachandran outliers		0.3%
Sidechain outliers		2.2%
RSRZ outliers		0

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	304	73% 25% ••
1	B	304	79% 18% •
1	D	304	76% 21% ••
2	C	304	73% 24% ••

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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	KPI	C	165	-	-	X	-
3	SI3	A	1165	X	-	-	-
3	SI3	B	1165	X	-	-	-
3	SI3	D	1165	X	-	-	-
5	MN9	C	1297	-	-	X	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 9360 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 N-ACETYLNEURAMINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total 2306	C 1466	N 396	O 434	S 10	0	0	0
1	B	295	Total 2272	C 1446	N 386	O 430	S 10	0	0	0
1	D	298	Total 2301	C 1464	N 394	O 433	S 10	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP P0A6L4
A	-5	GLU	-	expression tag	UNP P0A6L4
A	-4	HIS	-	expression tag	UNP P0A6L4
A	-3	HIS	-	expression tag	UNP P0A6L4
A	-2	HIS	-	expression tag	UNP P0A6L4
A	-1	HIS	-	expression tag	UNP P0A6L4
A	0	HIS	-	expression tag	UNP P0A6L4
A	1	HIS	-	expression tag	UNP P0A6L4
A	137	ALA	TYR	engineered mutation	UNP P0A6L4
B	-6	MET	-	expression tag	UNP P0A6L4
B	-5	GLU	-	expression tag	UNP P0A6L4
B	-4	HIS	-	expression tag	UNP P0A6L4
B	-3	HIS	-	expression tag	UNP P0A6L4
B	-2	HIS	-	expression tag	UNP P0A6L4
B	-1	HIS	-	expression tag	UNP P0A6L4
B	0	HIS	-	expression tag	UNP P0A6L4
B	1	HIS	-	expression tag	UNP P0A6L4
B	137	ALA	TYR	engineered mutation	UNP P0A6L4
D	-6	MET	-	expression tag	UNP P0A6L4
D	-5	GLU	-	expression tag	UNP P0A6L4
D	-4	HIS	-	expression tag	UNP P0A6L4
D	-3	HIS	-	expression tag	UNP P0A6L4
D	-2	HIS	-	expression tag	UNP P0A6L4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	HIS	-	expression tag	UNP P0A6L4
D	0	HIS	-	expression tag	UNP P0A6L4
D	1	HIS	-	expression tag	UNP P0A6L4
D	137	ALA	TYR	engineered mutation	UNP P0A6L4

- Molecule 2 is a protein called N-ACETYLNEURAMINATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	296	2287	1455	389	433	10	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	MET	-	expression tag	UNP P0A6L4
C	-5	GLU	-	expression tag	UNP P0A6L4
C	-4	HIS	-	expression tag	UNP P0A6L4
C	-3	HIS	-	expression tag	UNP P0A6L4
C	-2	HIS	-	expression tag	UNP P0A6L4
C	-1	HIS	-	expression tag	UNP P0A6L4
C	0	HIS	-	expression tag	UNP P0A6L4
C	1	HIS	-	expression tag	UNP P0A6L4
C	137	ALA	TYR	engineered mutation	UNP P0A6L4

- Molecule 3 is 5-(acetylamino)-3,5-dideoxy-D-glycero-D-galacto-non-2-ulosonic acid (three-letter code: SI3) (formula: $C_{11}H_{19}NO_9$).
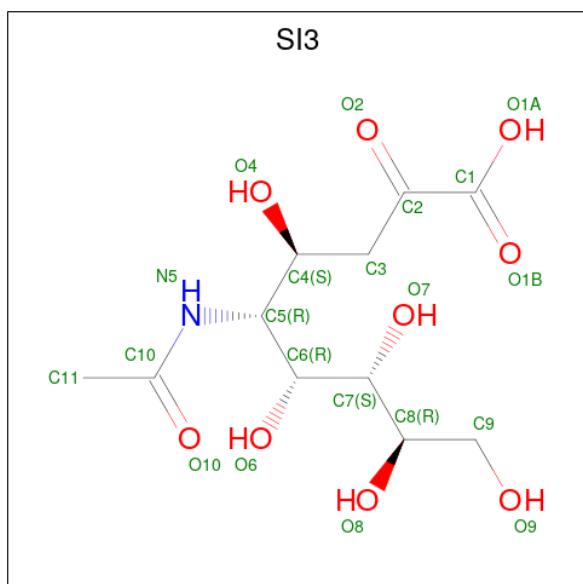
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 20	C 11	N 1	O 8	0	0
3	B	1	Total 20	C 11	N 1	O 8	0	0
3	D	1	Total 20	C 11	N 1	O 8	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).
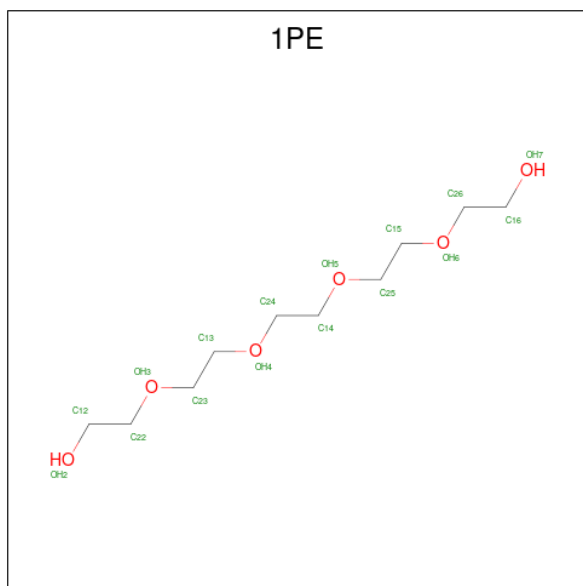
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 9	C 6	O 3	0	0
4	C	1	Total 8	C 5	O 3	0	0

- Molecule 5 is 2-(ACETYLAMINO)-2-DEOXY-D-MANNOSE (three-letter code: MN9) (formula: $C_8H_{15}NO_6$).

MN9

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	15	8	1	6	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	34	Total 34	O 34	0	0
6	B	22	Total 22	O 22	0	0
6	C	22	Total 22	O 22	0	0
6	D	24	Total 24	O 24	0	0

3   Residue-property plots ⓘ

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.
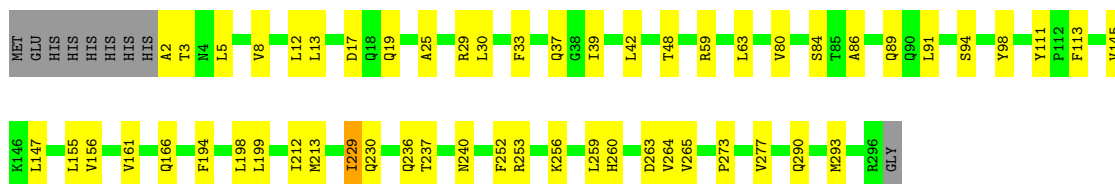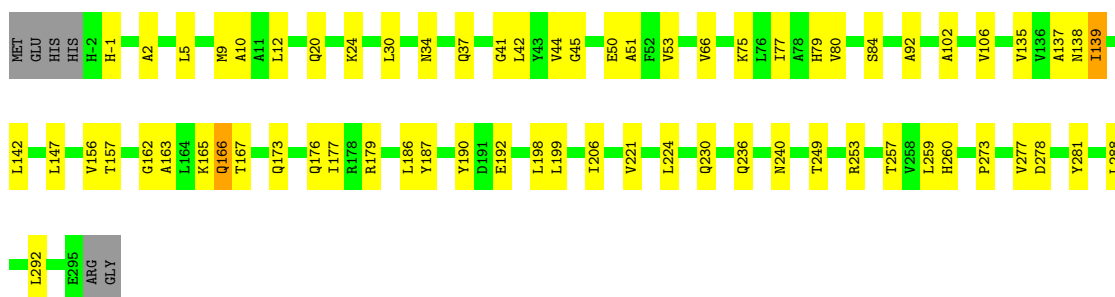
- Molecule 1: N-ACETYLNEURAMINATE LYASE

Chain A:
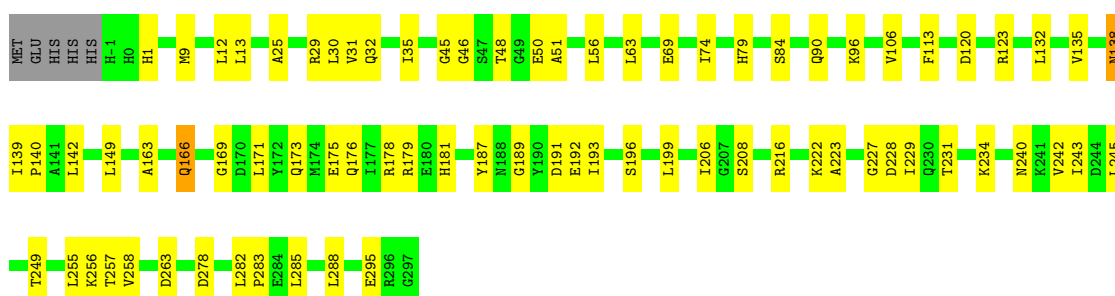
- Molecule 1: N-ACETYLNEURAMINATE LYASE

Chain B:

- Molecule 1: N-ACETYLNEURAMINATE LYASE

Chain D:

- Molecule 2: N-ACETYLNEURAMINATE LYASE

Chain C:

73%   24%

MET GLU HIS HIS HIS HIS HIS H1 A2 T3 A11 L12 L13 Q18 Q19 Q20 Q32 Q36 G41 L42 Y43 V44 G45 G46 V53 L56 Q61 V62 L63 E64 I65 V66 I74 H79 V80 L91 K96 A105 V106 T107 P108 F113 H118 D130

G131 L132 V135 N138 I139 P140 V156 V161 G162 A163 L164 K165 Q166 L171 Y172 Q173 Q176 Y187 N188 G189 Y190 D191 E192 I193 F194 A195 S196 G197 L198 I206 Q207 S208 T209 Y210 N211 W215 G227 D228 I229 Q233 Q236 T237 N240 D244 L245 L246

T249 L255 Y261 M262 D263 V264 K272 L282 L285 Q291 L292 R296 GLY

4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.97Å 143.22Å 83.41Å 90.00° 109.51° 90.00°	Depositor
Resolution (Å)	49.46 – 2.00 49.50 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.46-2.00) 99.4 (49.50-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0097	Depositor
R, R_{free}	0.180 , 0.235 0.186 , 0.228	Depositor DCC
R_{free} test set	4145 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	26.2	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 31.9	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.107 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.512 for H, K, L 0.488 for -H, -K, H+L	Depositor
Outliers	0 of 83318 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9360	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, SI3, KPI, MN9

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	0.53	0/2348	0.65	0/3178
1	B	0.56	0/2311	0.66	0/3128
1	D	0.58	0/2344	0.67	0/3174
2	C	0.57	0/2312	0.68	0/3129
All	All	0.56	0/9315	0.67	0/12609

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	2306	0	2320	57	0
1	B	2272	0	2293	35	0
1	D	2301	0	2312	51	0
2	C	2287	0	2305	66	0
3	A	20	0	18	2	0
3	B	20	0	18	0	0
3	D	20	0	18	1	0
4	B	9	0	10	0	0
4	C	8	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	15	0	15	8	0
6	A	34	0	0	0	0
6	B	22	0	0	1	0
6	C	22	0	0	1	0
6	D	24	0	0	2	0
All	All	9360	0	9318	199	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 11.

The worst 5 of 199 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:C:165:KPI:C1	5:C:1297:MN9:H	1.74	1.16
1:B:2:ALA:HB1	1:B:5:LEU:HD12	1.36	1.07
1:D:139:ILE:HD11	1:D:142:LEU:HD12	1.37	1.05
2:C:165:KPI:H1B	5:C:1297:MN9:H	1.36	1.03
2:C:165:KPI:H1A	2:C:206:ILE:HG22	1.42	0.97

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	297/304 (98%)	282 (95%)	13 (4%)	2 (1%)	22	16
1	B	293/304 (96%)	277 (94%)	15 (5%)	1 (0%)	41	37
1	D	296/304 (97%)	287 (97%)	9 (3%)	0	100	100
2	C	293/304 (96%)	279 (95%)	14 (5%)	0	100	100
All	All	1179/1216 (97%)	1125 (95%)	51 (4%)	3 (0%)	41	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ASP
1	B	37	GLN
1	A	1	HIS

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	245/250 (98%)	239 (98%)	6 (2%)	49	51
1	B	242/250 (97%)	237 (98%)	5 (2%)	53	57
1	D	245/250 (98%)	240 (98%)	5 (2%)	55	58
2	C	242/249 (97%)	237 (98%)	5 (2%)	53	57
All	All	974/999 (98%)	953 (98%)	21 (2%)	52	55

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

Mol	Chain	Res	Type
2	C	138	ASN
1	D	139	ILE
1	D	230	GLN
1	D	157	THR
1	D	84	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	181	HIS
1	D	138	ASN
2	C	233	GLN
1	D	37	GLN
1	D	166	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	KPI	C	165	2	11,13,14	1.00	0	10,15,17	1.45	2 (20%)

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	KPI	C	165	2	-	0/13/14/16	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	165	KPI	O2-CX2-CX1	-3.09	117.43	121.38
2	C	165	KPI	C1-CX1-CX2	2.23	120.33	118.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	165	KPI	11	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	$\#|Z| > 2$
3	SI3	D	1165	1	19,19,20	1.97	3 (15%)	20,25,27	1.38	4 (20%)
4	1PE	C	1298	-	7,7,15	0.71	0	6,6,14	0.43	0
3	SI3	A	1165	1	19,19,20	2.00	4 (21%)	20,25,27	1.27	2 (10%)
3	SI3	B	1165	1	19,19,20	1.80	3 (15%)	20,25,27	1.56	4 (20%)
5	MN9	C	1297	-	13,14,14	0.65	0	14,18,18	1.37	2 (14%)
4	1PE	B	1297	-	8,8,15	0.81	0	7,7,14	0.61	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	SI3	D	1165	1	1/1/7/9	12/27/27/30	-
4	1PE	C	1298	-	-	3/5/5/13	-
3	SI3	A	1165	1	1/1/7/9	8/27/27/30	-
3	SI3	B	1165	1	1/1/7/9	7/27/27/30	-
5	MN9	C	1297	-	-	6/18/20/20	-
4	1PE	B	1297	-	-	5/6/6/13	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1165	SI3	O1B-C1	6.61	1.44	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1165	SI3	O1B-C1	6.59	1.44	1.22
3	B	1165	SI3	O1B-C1	6.34	1.43	1.22
3	D	1165	SI3	C10-N5	3.61	1.46	1.34
3	B	1165	SI3	C10-N5	3.23	1.45	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1165	SI3	C3-C2-C1	3.63	122.15	112.51
3	B	1165	SI3	C8-C7-C6	3.48	117.92	112.47
5	C	1297	MN9	C2-N2-C7	3.35	126.78	123.12
3	B	1165	SI3	C3-C2-C1	2.91	120.24	112.51
3	D	1165	SI3	C3-C2-C1	2.84	120.04	112.51

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1165	SI3	C4
3	B	1165	SI3	C4
3	D	1165	SI3	C4

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1165	SI3	C1-C2-C3-C4
3	A	1165	SI3	C3-C4-C5-N5
3	A	1165	SI3	C3-C4-C5-C6
3	B	1165	SI3	C2-C3-C4-C5
3	B	1165	SI3	C3-C4-C5-N5

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1165	SI3	1	0
3	A	1165	SI3	2	0
5	C	1297	MN9	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

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

Ligand SI3 D 1165

Bond lengths

Bond angles

Torsions

Rings

Ligand SI3 A 1165

Bond lengths

Bond angles

Torsions

Rings

Ligand SI3 B 1165

Bond lengths

Bond angles

Torsions

Rings
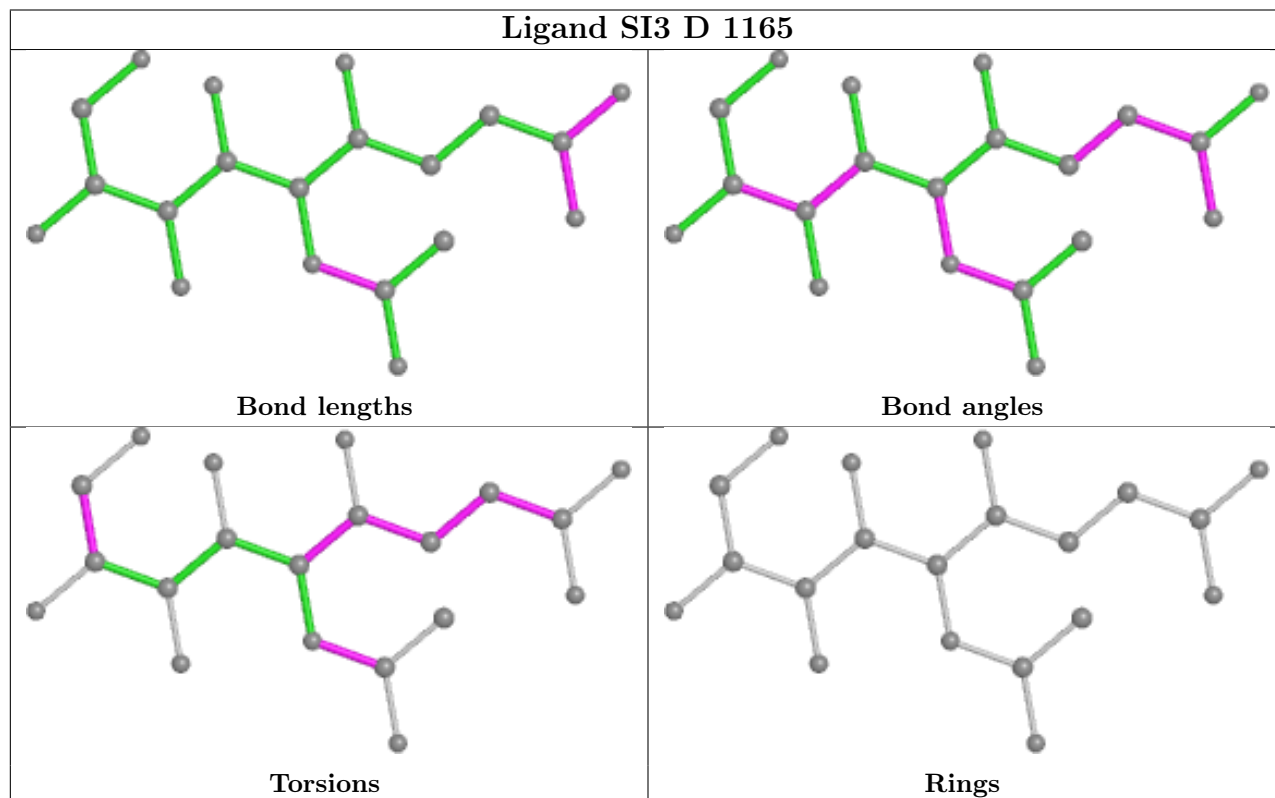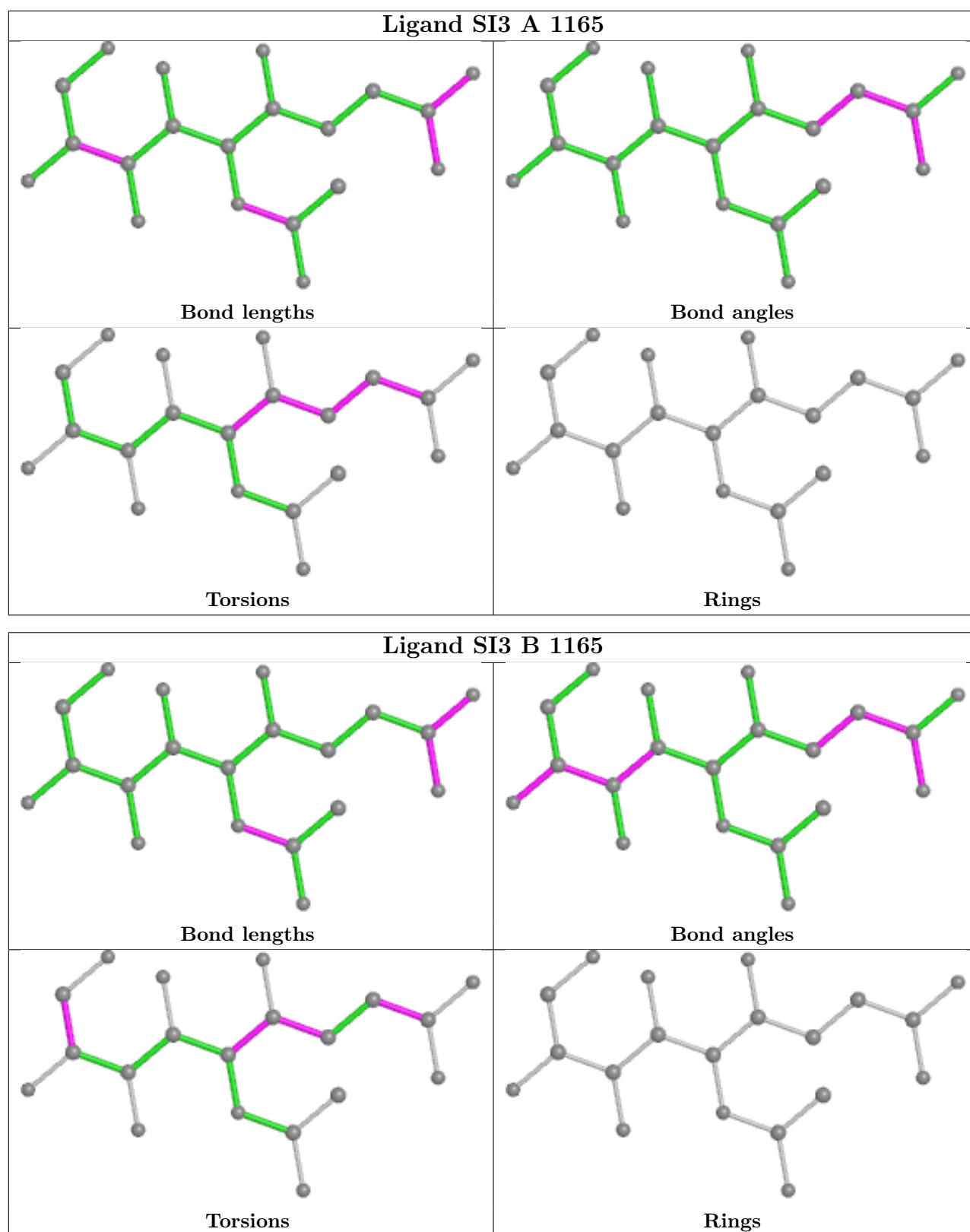
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	299/304 (98%)	-0.55	0	100	100	18, 28, 44, 58	4 (1%)
1	B	295/304 (97%)	-0.54	0	100	100	17, 27, 36, 44	4 (1%)
1	D	298/304 (98%)	-0.66	0	100	100	16, 25, 35, 52	1 (0%)
2	C	295/304 (97%)	-0.48	0	100	100	17, 25, 38, 46	0
All	All	1187/1216 (97%)	-0.56	0	100	100	16, 26, 39, 58	9 (0%)

There are no RSRZ outliers to report.

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

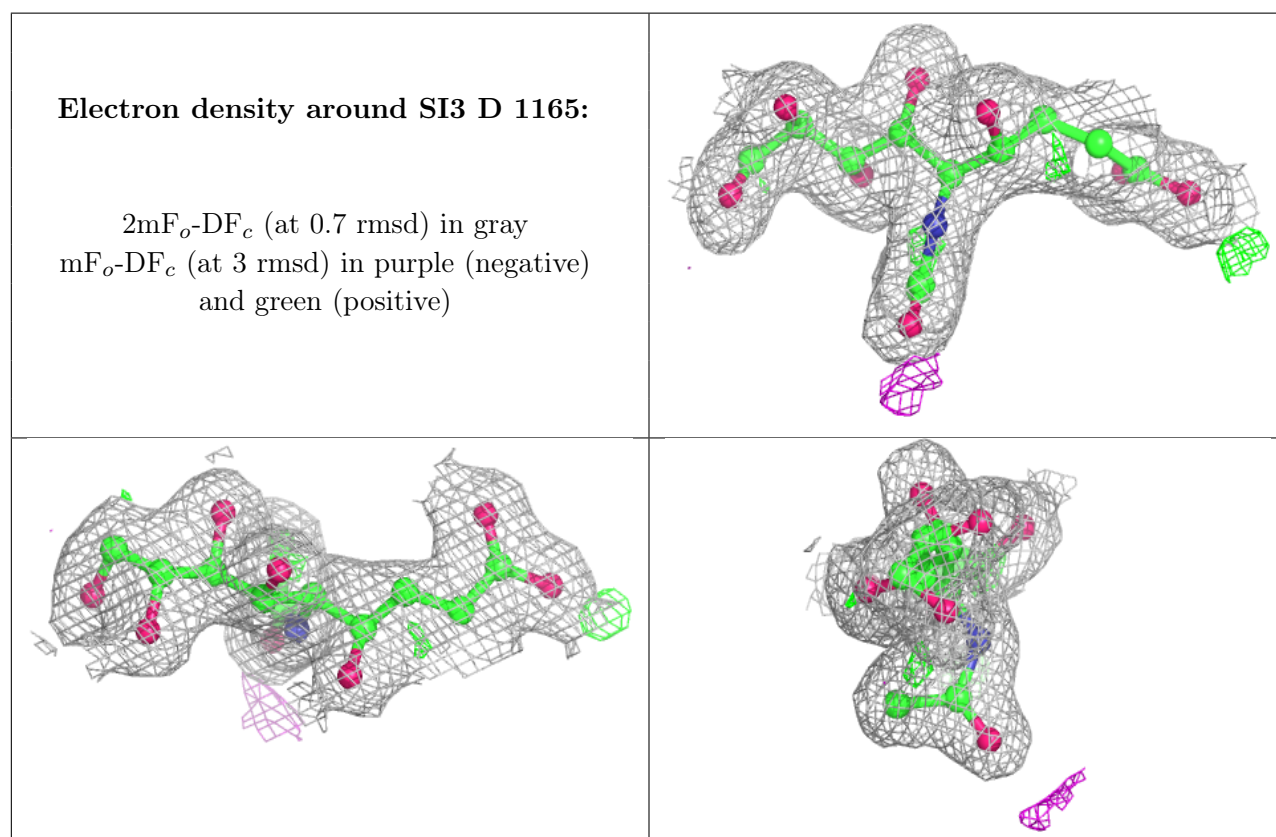| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	KPI	C	165	14/15	0.96	0.11	16,20,28,30	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

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	1PE	B	1297	9/16	0.93	0.12	24,30,33,34	0
3	SI3	D	1165	20/21	0.94	0.08	20,24,27,29	0
3	SI3	B	1165	20/21	0.95	0.09	19,26,31,33	0
4	1PE	C	1298	8/16	0.95	0.14	38,39,41,42	0
3	SI3	A	1165	20/21	0.96	0.08	20,25,31,31	0
5	MN9	C	1297	15/15	0.97	0.09	13,25,28,31	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.
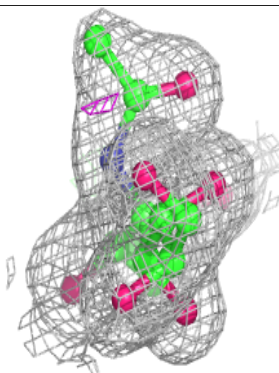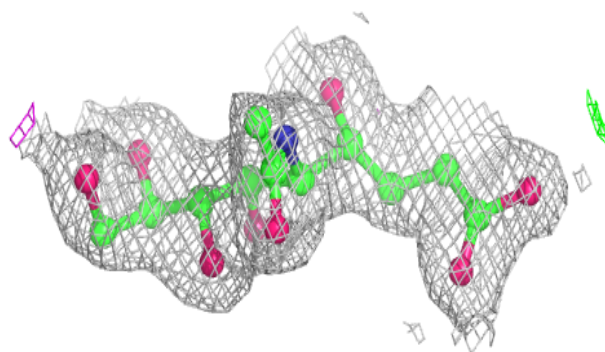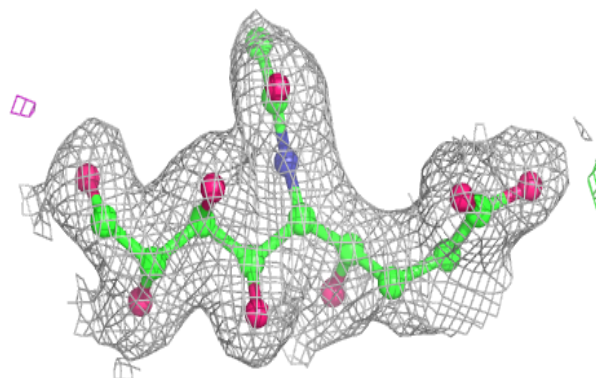

Electron density around SI3 D 1165:

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 SI3 B 1165:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
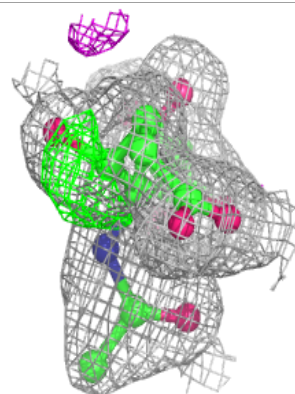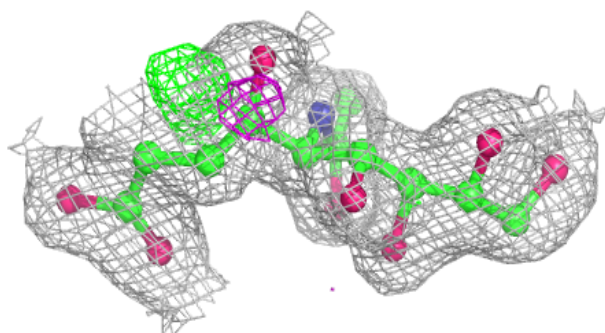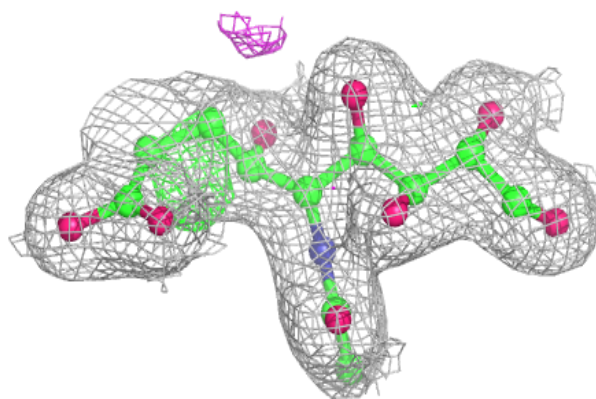
Electron density around SI3 A 1165:

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.