wwPDB X-ray Structure Validation Summary Report (i)

Aug 24, 2023 – 10:18 AM JST

PDB ID	:	8HRH
Title	:	SN-131/1B2 anti-MUC1 antibody with a glycopeptide
Authors	:	Wakui, H.; Horidome, C.; Yao, M.; Ose, T.; Nishimura, S.-I.
Deposited on	:	2022-12-15
Resolution	:	2.07 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 (i) 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 (i)) were used in the production of this report:

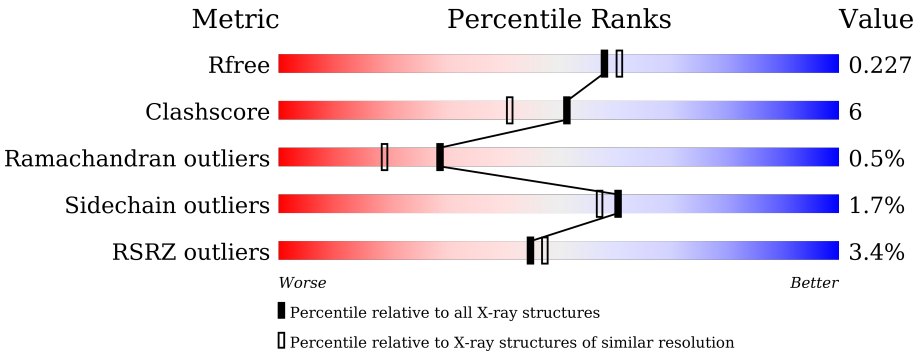
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.07 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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	467	3%, 38%, 7%, 54%
2	B	238	80%, 10%, 8%
3	D	3	33%, 67%

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 3711 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.

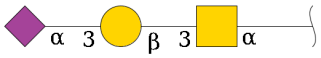
- Molecule 1 is a protein called Heavy chain of SN-131/1B2 antibody Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1612	1021	271	315	5	0	0	0

- Molecule 2 is a protein called Light chain of SN-131/1B2 antibody Fab.

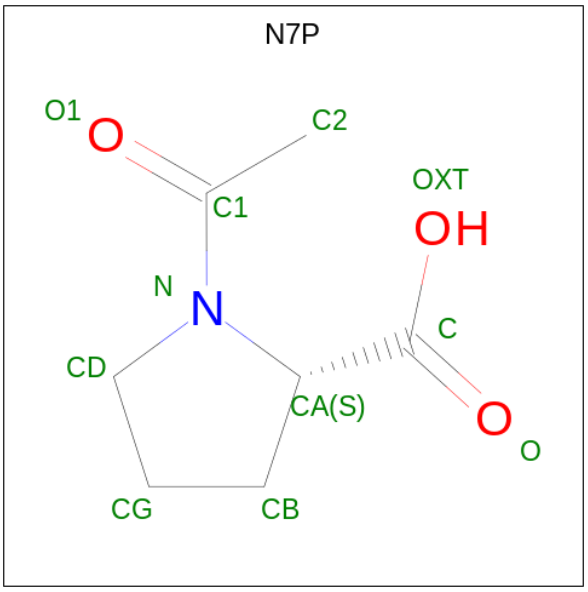
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	218	1716	1082	287	341	6	0	0	0

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose.



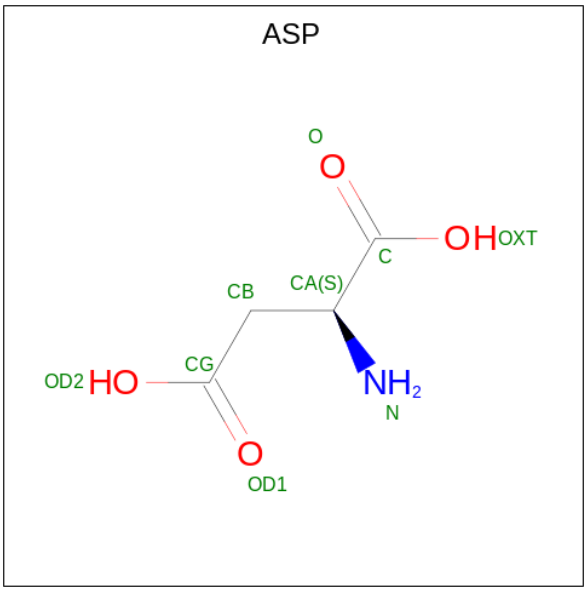
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	3	45	25	2	18	0	0	0

- Molecule 4 is 1-ACETYL-L-PROLINE (three-letter code: N7P) (formula: $C_7H_{11}NO_3$) (labeled as "Ligand of Interest" by depositor).



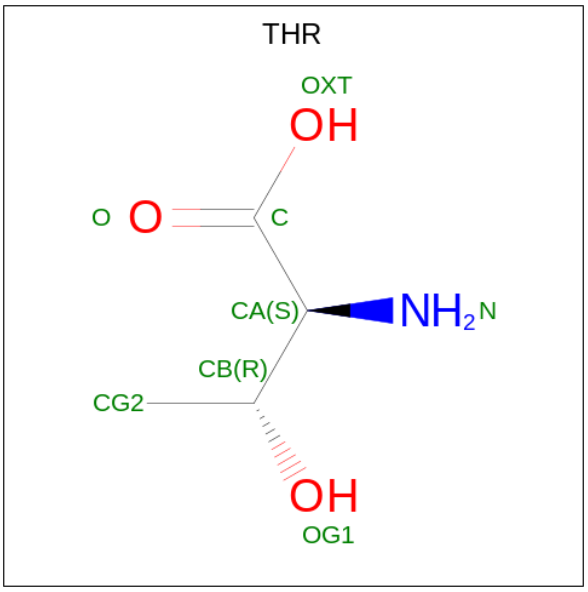
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	10	7	1	2	0	0

- Molecule 5 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$) (labeled as "Ligand of Interest" by depositor).



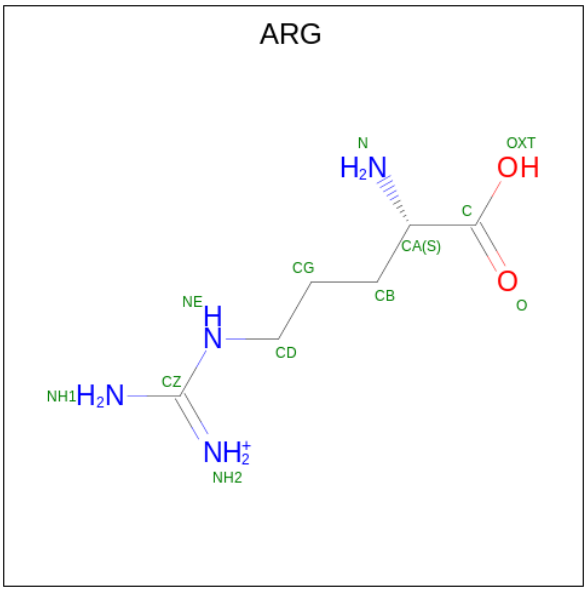
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	8	4	1	3	0	0

- Molecule 6 is THREONINE (three-letter code: THR) (formula: $C_4H_9NO_3$) (labeled as "Ligand of Interest" by depositor).



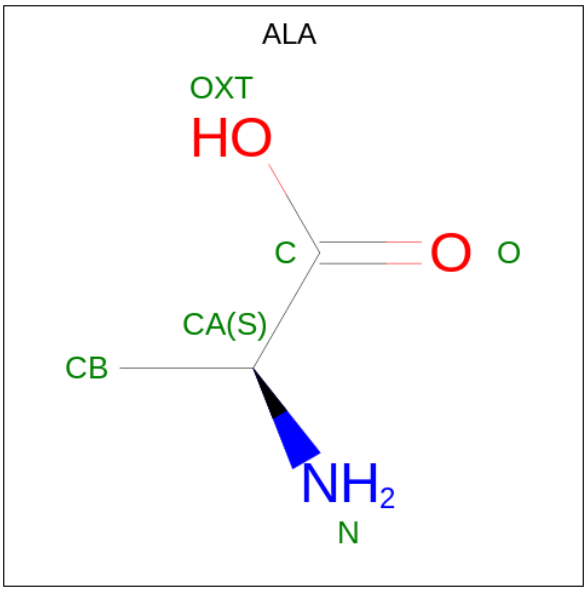
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	7	4	1	2	0	0

- Molecule 7 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



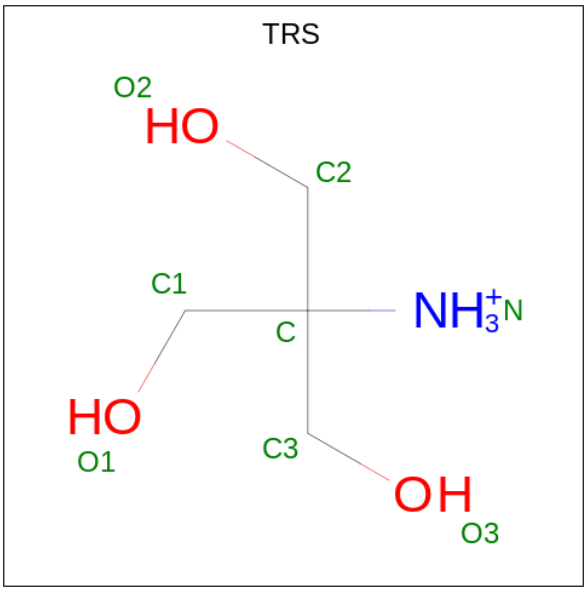
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	11	6	4	1	0	0

- Molecule 8 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$) (labeled as "Ligand of Interest" by depositor).



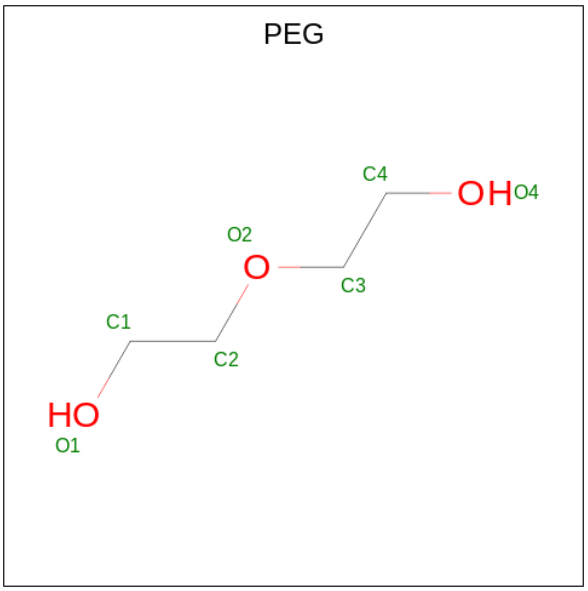
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	5	3	1	1	0	0

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



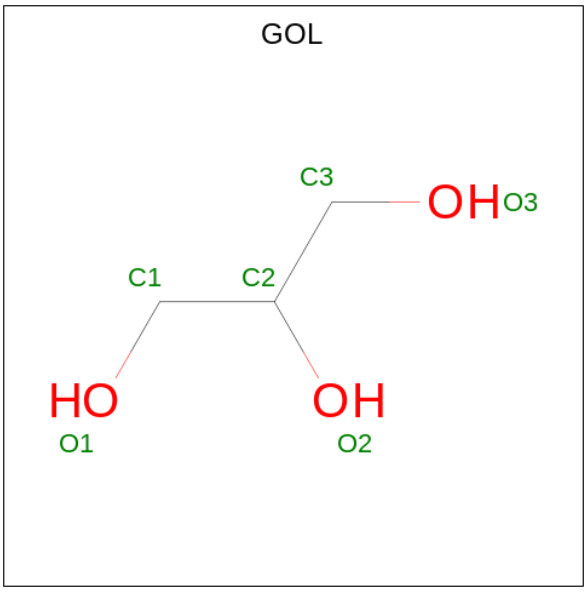
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	A	1	8	4	1	3	0	0

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



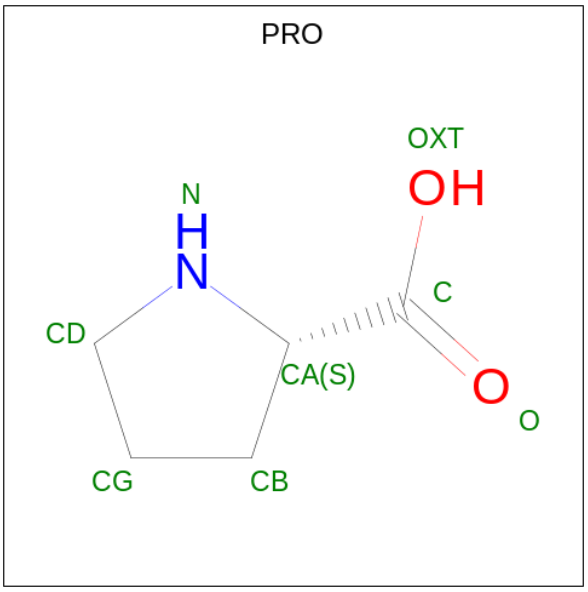
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 7 4 3	0	0
10	A	1	Total C O 7 4 3	0	0
10	B	1	Total C O 7 4 3	0	0
10	B	1	Total C O 7 4 3	0	0
10	B	1	Total C O 7 4 3	0	0
10	B	1	Total C O 7 4 3	0	0
10	B	1	Total C O 7 4 3	0	0

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



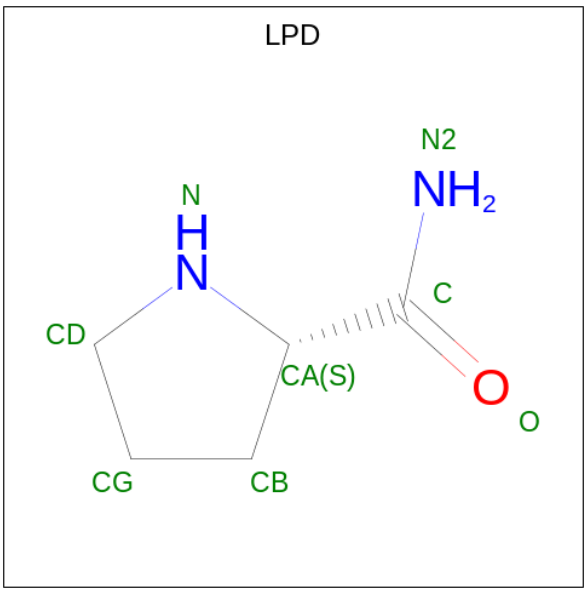
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O 6 3 3	0	0
11	A	1	Total C O 6 3 3	0	0

- Molecule 12 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C N O 7 5 1 1	0	0

- Molecule 13 is L-PROLINAMIDE (three-letter code: LPD) (formula: $C_5H_{10}N_2O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total C N O 8 5 2 1	0	0

- Molecule 14 is water.

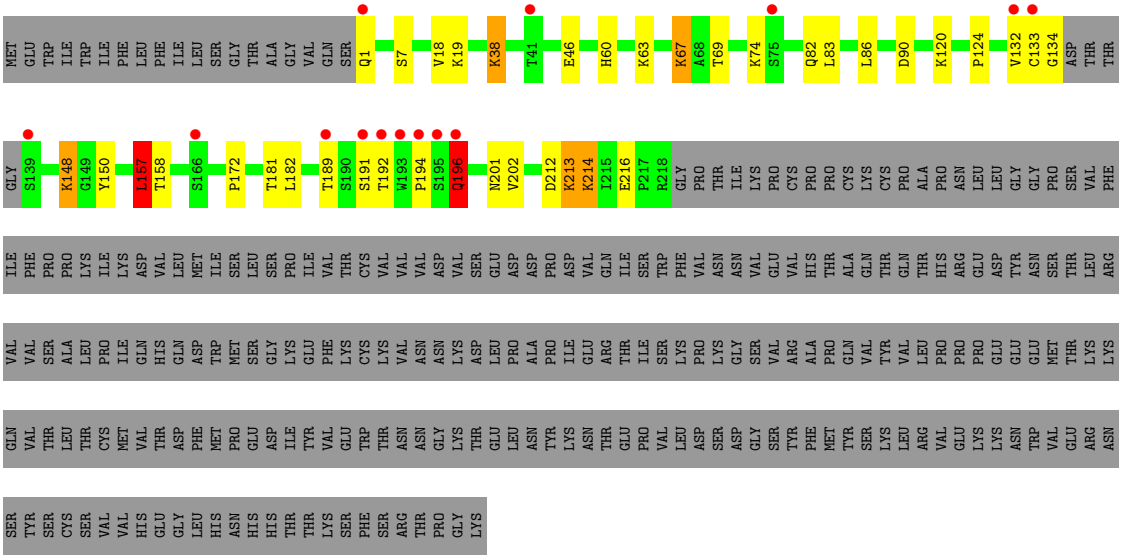
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	94	Total O 94 94	0	0
14	B	119	Total O 119 119	0	0

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.

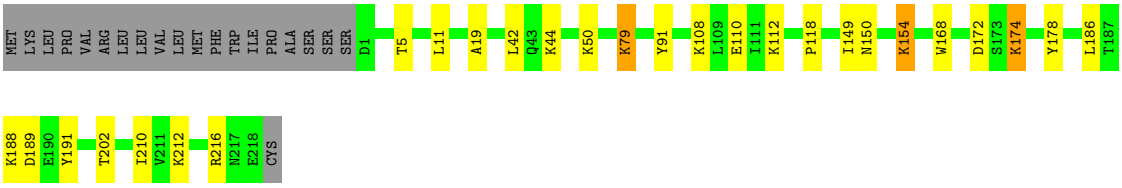
• Molecule 1: Heavy chain of SN-131/1B2 antibody Fab

Chain A:



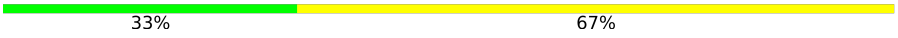
• Molecule 2: Light chain of SN-131/1B2 antibody Fab

Chain B:



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	84.59Å 84.59Å 271.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.77 – 2.07 49.77 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.77-2.07) 99.9 (49.77-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.16-3549	Depositor
R, R_{free}	0.192 , 0.227 0.192 , 0.227	Depositor DCC
R_{free} test set	1804 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.4	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3711	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: N7P, TRS, GAL, PEG, A2G, GOL, SIA, MLY, LPD

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	0.32	0/1562	0.55	1/2139 (0.0%)
2	B	0.32	0/1624	0.52	0/2218
All	All	0.32	0/3186	0.53	1/4357 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	157	LEU	CA-CB-CG	5.90	128.86	115.30

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	1612	0	1585	24	0
2	B	1716	0	1656	13	0
3	D	45	0	37	0	0
4	A	10	0	0	0	0
5	A	8	0	4	0	0
6	A	7	0	6	0	0
7	A	11	0	13	0	0
8	A	5	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	8	0	12	1	0
10	A	14	0	20	2	0
10	B	35	0	50	3	0
11	A	12	0	16	4	0
12	B	7	0	7	0	0
13	B	8	0	9	0	0
14	A	94	0	0	4	0
14	B	119	0	0	1	0
All	All	3711	0	3419	39	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 6.

The worst 5 of 39 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)
11:A:510:GOL:HO3	11:A:510:GOL:HO1	1.23	0.83
2:B:108:LYS:HB2	10:B:306:PEG:H32	1.66	0.77
1:A:157:LEU:HD22	1:A:202:VAL:HG22	1.75	0.66
2:B:172:ASP:OD2	2:B:174:MLY:HH22	1.97	0.64
2:B:5:THR:HG21	10:B:305:PEG:H11	1.85	0.59

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	202/467 (43%)	194 (96%)	6 (3%)	2 (1%)	15 6
2	B	204/238 (86%)	198 (97%)	6 (3%)	0	100 100
All	All	406/705 (58%)	392 (97%)	12 (3%)	2 (0%)	29 19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	CYS
1	A	196	GLN

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	170/405 (42%)	166 (98%)	4 (2%)	49	43
2	B	182/201 (90%)	180 (99%)	2 (1%)	73	72
All	All	352/606 (58%)	346 (98%)	6 (2%)	60	57

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
2	B	186	LEU
2	B	189	ASP
1	A	182	LEU
1	A	157	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

20 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	MLY	A	213	1	9,10,11	0.99	1 (11%)	6,11,13	0.72	0
1	MLY	A	214	1	9,10,11	1.01	1 (11%)	6,11,13	0.60	0
2	MLY	B	55	2	9,10,11	0.91	0	6,11,13	0.62	0
2	MLY	B	188	2	9,10,11	0.93	1 (11%)	6,11,13	0.86	0
1	MLY	A	38	1	9,10,11	0.97	1 (11%)	6,11,13	1.06	0
1	MLY	A	67	1	9,10,11	0.95	1 (11%)	6,11,13	0.80	0
2	MLY	B	212	2	9,10,11	0.91	1 (11%)	6,11,13	0.78	0
2	MLY	B	79	2	9,10,11	0.94	1 (11%)	6,11,13	0.65	0
2	MLY	B	50	2	9,10,11	0.89	1 (11%)	6,11,13	0.93	0
1	MLY	A	148	1	9,10,11	1.02	1 (11%)	6,11,13	0.90	0
2	MLY	B	152	2	9,10,11	0.91	0	6,11,13	0.75	0
2	MLY	B	112	2	9,10,11	0.96	1 (11%)	6,11,13	0.94	0
2	MLY	B	204	2	9,10,11	0.95	0	6,11,13	0.55	0
2	MLY	B	174	2	9,10,11	0.98	1 (11%)	6,11,13	0.67	0
1	MLY	A	120	1	9,10,11	0.99	1 (11%)	6,11,13	0.74	0
1	MLY	A	19	1	9,10,11	0.95	1 (11%)	6,11,13	0.66	0
2	MLY	B	44	2	9,10,11	0.91	0	6,11,13	1.12	1 (16%)
1	MLY	A	74	1	9,10,11	0.94	1 (11%)	6,11,13	0.85	0
2	MLY	B	147	2	9,10,11	0.96	0	6,11,13	0.99	0
2	MLY	B	154	2	9,10,11	0.97	1 (11%)	6,11,13	0.66	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
1	MLY	A	213	1	-	5/8/9/11	-
1	MLY	A	214	1	-	0/8/9/11	-
2	MLY	B	55	2	-	2/8/9/11	-
2	MLY	B	188	2	-	4/8/9/11	-
1	MLY	A	38	1	-	2/8/9/11	-
1	MLY	A	67	1	-	1/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLY	B	212	2	-	0/8/9/11	-
2	MLY	B	79	2	-	5/8/9/11	-
2	MLY	B	50	2	-	2/8/9/11	-
1	MLY	A	148	1	-	4/8/9/11	-
2	MLY	B	152	2	-	1/8/9/11	-
2	MLY	B	112	2	-	2/8/9/11	-
2	MLY	B	204	2	-	2/8/9/11	-
2	MLY	B	174	2	-	3/8/9/11	-
1	MLY	A	120	1	-	1/8/9/11	-
1	MLY	A	19	1	-	1/8/9/11	-
2	MLY	B	44	2	-	2/8/9/11	-
1	MLY	A	74	1	-	3/8/9/11	-
2	MLY	B	147	2	-	0/8/9/11	-
2	MLY	B	154	2	-	5/8/9/11	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	MLY	CA-N	-2.30	1.41	1.48
2	B	112	MLY	CA-N	-2.30	1.41	1.48
1	A	214	MLY	CA-N	-2.28	1.41	1.48
2	B	154	MLY	CA-N	-2.23	1.41	1.48
1	A	213	MLY	CA-N	-2.20	1.41	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	44	MLY	CD-CE-NZ	-2.07	108.18	113.79

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	38	MLY	N-CA-CB-CG
1	A	213	MLY	N-CA-CB-CG
1	A	213	MLY	C-CA-CB-CG
2	B	50	MLY	C-CA-CB-CG
2	B	112	MLY	C-CA-CB-CG

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	213	MLY	1	0
1	A	214	MLY	1	0
1	A	38	MLY	1	0
1	A	67	MLY	1	0
2	B	79	MLY	1	0
1	A	148	MLY	3	0
2	B	174	MLY	2	0
2	B	154	MLY	1	0

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	$\#\|Z\| > 2$
3	A2G	D	1	3,6	14,14,15	0.25	0	17,19,21	1.05	1 (5%)
3	GAL	D	2	3	11,11,12	0.22	0	15,15,17	0.67	0
3	SIA	D	3	3	20,20,21	0.51	0	24,28,31	1.03	2 (8%)

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	A2G	D	1	3,6	-	0/6/23/26	0/1/1/1
3	GAL	D	2	3	-	0/2/19/22	0/1/1/1
3	SIA	D	3	3	-	3/18/34/38	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1	A2G	C1-O5-C5	2.82	116.02	112.19
3	D	3	SIA	O6-C2-C1	2.49	112.58	107.70
3	D	3	SIA	O1B-C1-C2	2.44	119.99	113.03

There are no chirality outliers.

All (3) torsion outliers are listed below:

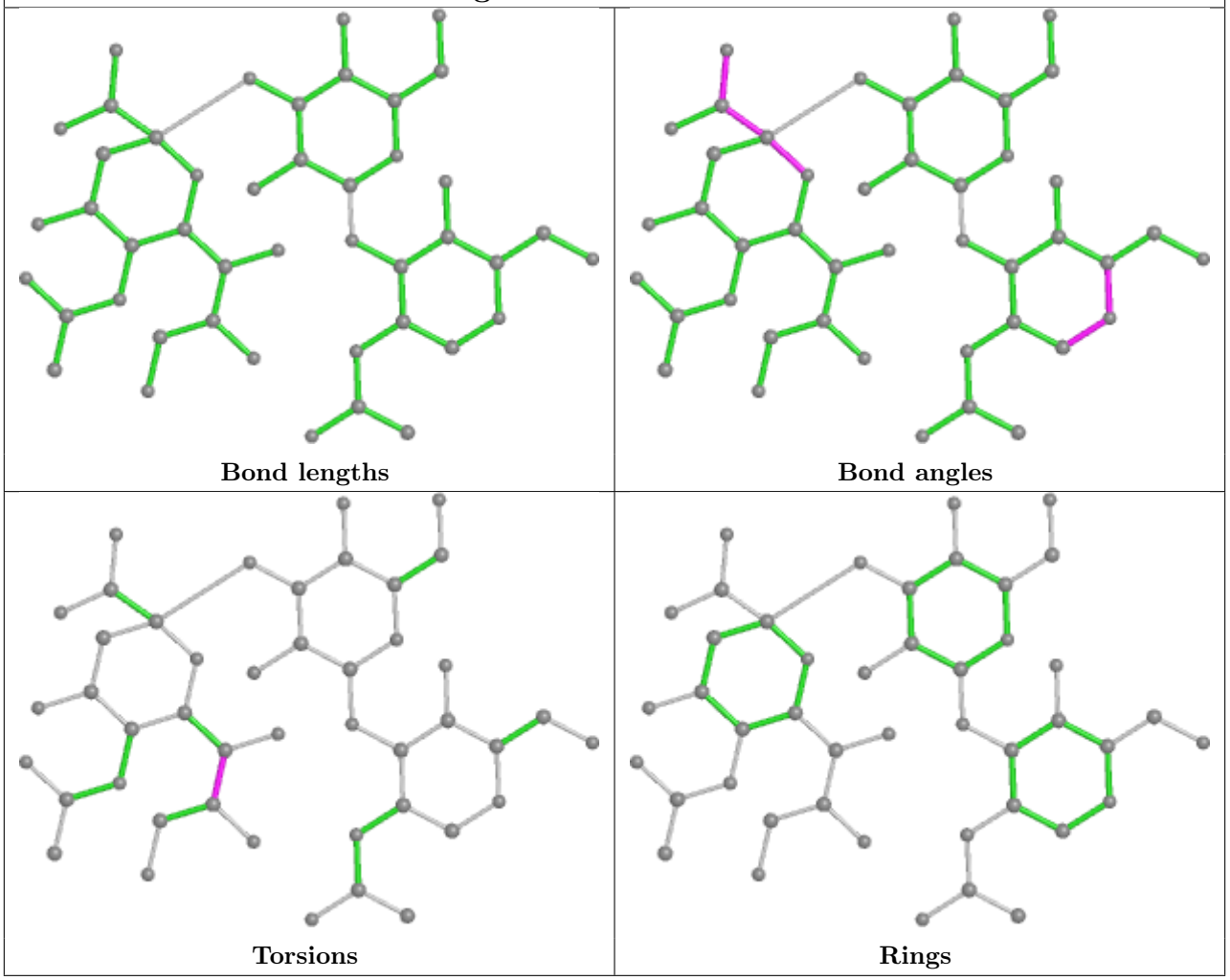
Mol	Chain	Res	Type	Atoms
3	D	3	SIA	C6-C7-C8-O8
3	D	3	SIA	O7-C7-C8-O8
3	D	3	SIA	O7-C7-C8-C9

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.

Oligosaccharide Chain D



5.6 Ligand geometry (i)

17 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	N7P	A	501	5	9,10,11	1.46	1 (11%)	9,13,15	1.79	3 (33%)
7	ARG	A	504	12	9,10,11	0.52	0	5,11,13	0.91	0
9	TRS	A	506	-	7,7,7	0.53	0	9,9,9	0.39	0
10	PEG	A	507	-	6,6,6	0.49	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	PEG	B	305	-	6,6,6	0.48	0	5,5,5	0.19	0
11	GOL	A	510	-	5,5,5	0.80	0	5,5,5	0.78	0
10	PEG	A	508	-	6,6,6	0.47	0	5,5,5	0.34	0
6	THR	A	503	3	5,6,7	0.55	0	6,7,9	0.79	0
10	PEG	B	307	-	6,6,6	0.51	0	5,5,5	0.26	0
12	PRO	B	301	7,8	5,7,8	0.45	0	7,8,10	0.99	0
11	GOL	A	509	-	5,5,5	1.12	0	5,5,5	0.80	0
10	PEG	B	306	-	6,6,6	0.47	0	5,5,5	0.23	0
13	LPD	B	302	-	8,8,8	1.46	1 (12%)	10,10,10	1.20	0
8	ALA	A	505	12	3,4,5	0.68	0	2,4,6	0.85	0
5	ASP	A	502	4	6,7,8	0.97	0	5,8,10	0.70	0
10	PEG	B	304	-	6,6,6	0.49	0	5,5,5	0.35	0
10	PEG	B	303	-	6,6,6	0.49	0	5,5,5	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	N7P	A	501	5	-	0/4/16/18	0/1/1/1
7	ARG	A	504	12	-	1/8/9/11	-
9	TRS	A	506	-	-	0/9/9/9	-
10	PEG	A	507	-	-	1/4/4/4	-
10	PEG	B	305	-	-	1/4/4/4	-
11	GOL	A	510	-	-	2/4/4/4	-
10	PEG	A	508	-	-	1/4/4/4	-
6	THR	A	503	3	-	1/5/6/8	-
10	PEG	B	307	-	-	1/4/4/4	-
12	PRO	B	301	7,8	-	0/0/9/11	0/1/1/1
11	GOL	A	509	-	-	2/4/4/4	-
10	PEG	B	306	-	-	2/4/4/4	-
13	LPD	B	302	-	-	2/4/11/11	0/1/1/1
8	ALA	A	505	12	-	0/0/2/4	-
5	ASP	A	502	4	-	1/5/6/8	-
10	PEG	B	304	-	-	1/4/4/4	-
10	PEG	B	303	-	-	1/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	N7P	CA-N	-3.61	1.45	1.48
13	B	302	LPD	C-N2	3.61	1.42	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	N7P	C2-C1-N	4.00	122.06	117.87
4	A	501	N7P	CA-N-C1	2.31	126.93	121.26
4	A	501	N7P	CG-CD-N	2.07	106.88	103.25

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	502	ASP	O-C-CA-CB
7	A	504	ARG	O-C-CA-CB
13	B	302	LPD	O-C-CA-N
13	B	302	LPD	N2-C-CA-N
10	A	507	PEG	O2-C3-C4-O4

There are no ring outliers.

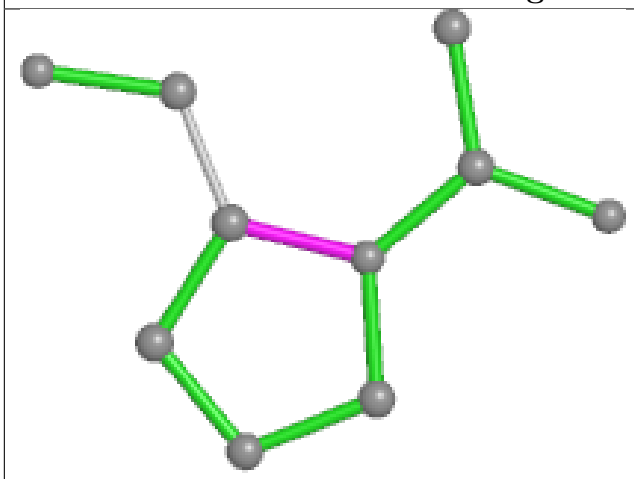
7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	506	TRS	1	0
10	A	507	PEG	2	0
10	B	305	PEG	1	0
11	A	510	GOL	2	0
10	B	307	PEG	1	0
11	A	509	GOL	2	0
10	B	306	PEG	1	0

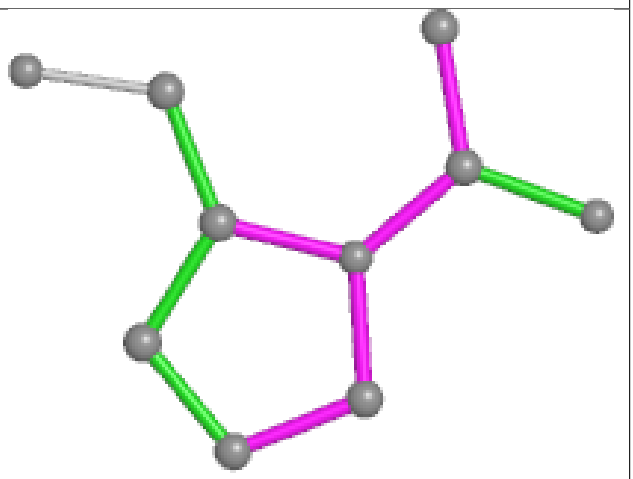
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

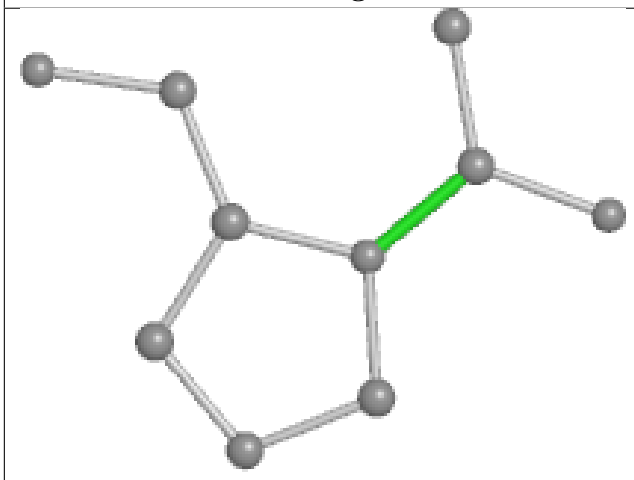
Ligand N7P A 501



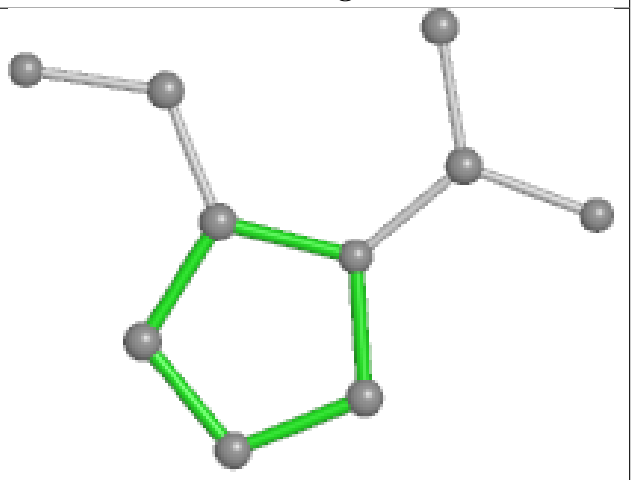
Bond lengths



Bond angles

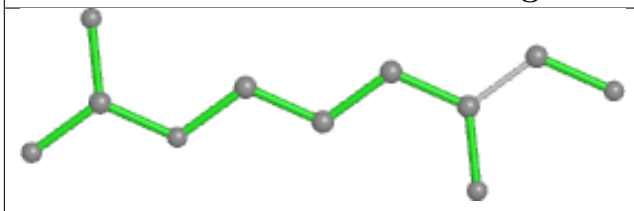


Torsions

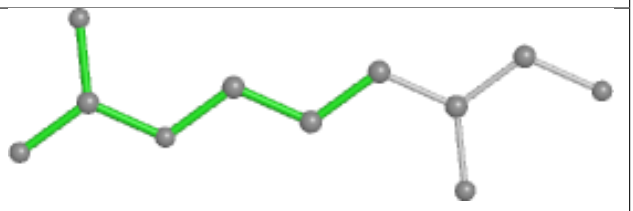


Rings

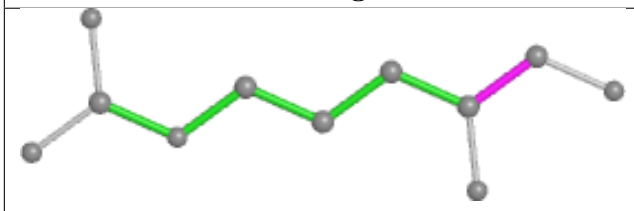
Ligand ARG A 504



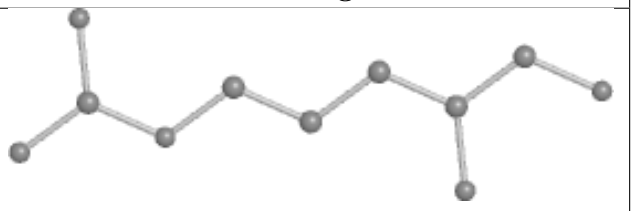
Bond lengths



Bond angles

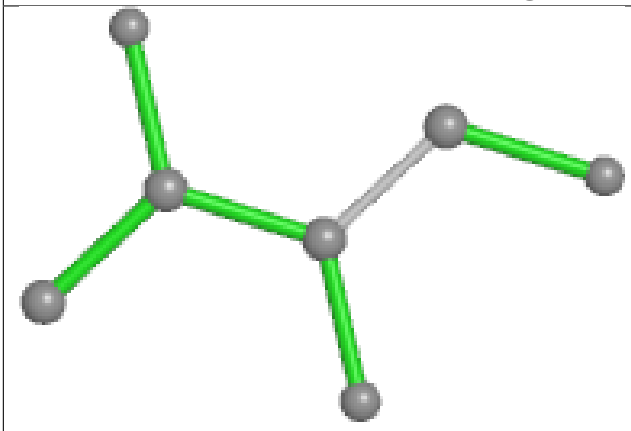


Torsions

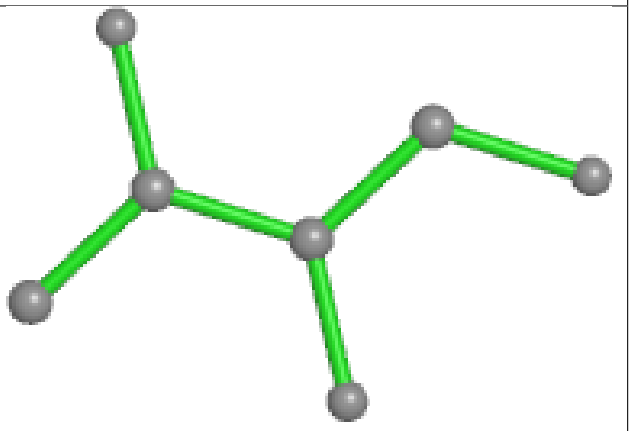


Rings

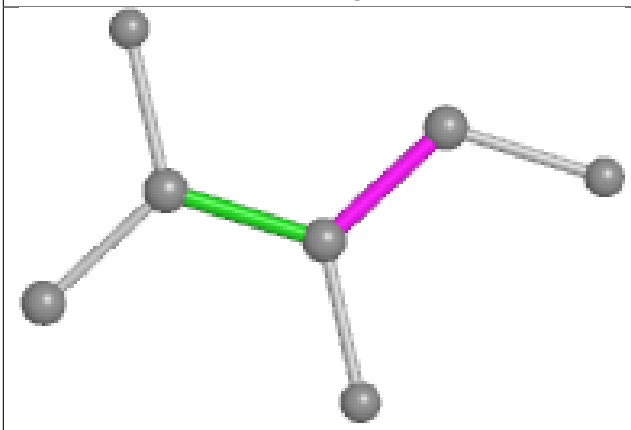
Ligand THR A 503



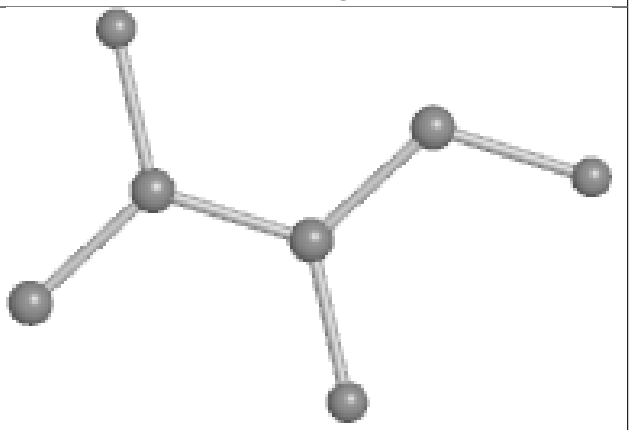
Bond lengths



Bond angles

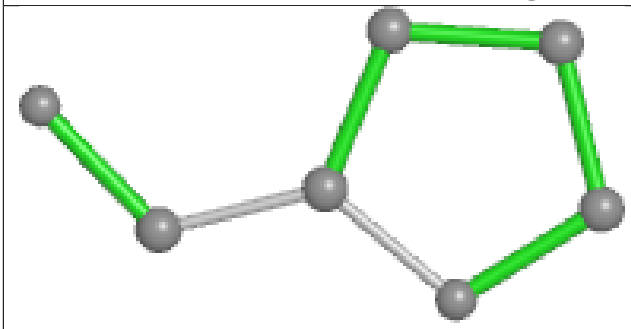


Torsions

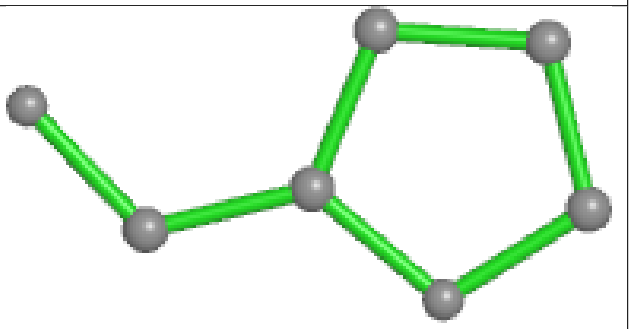


Rings

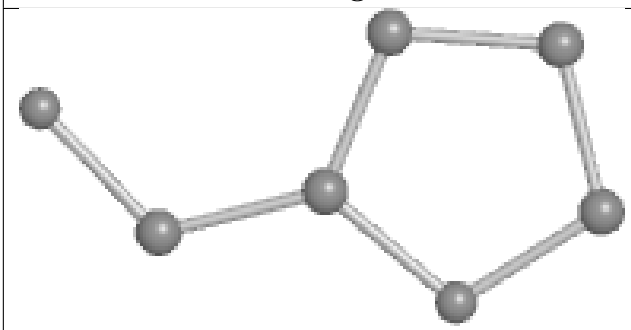
Ligand PRO B 301



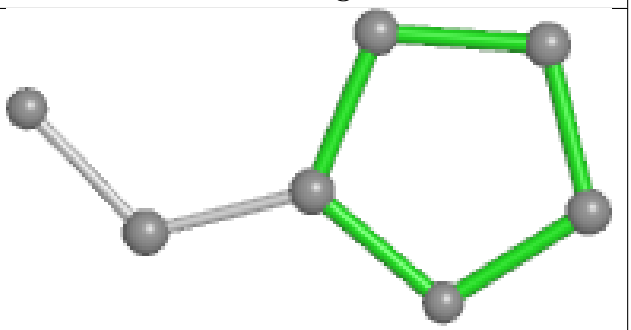
Bond lengths



Bond angles

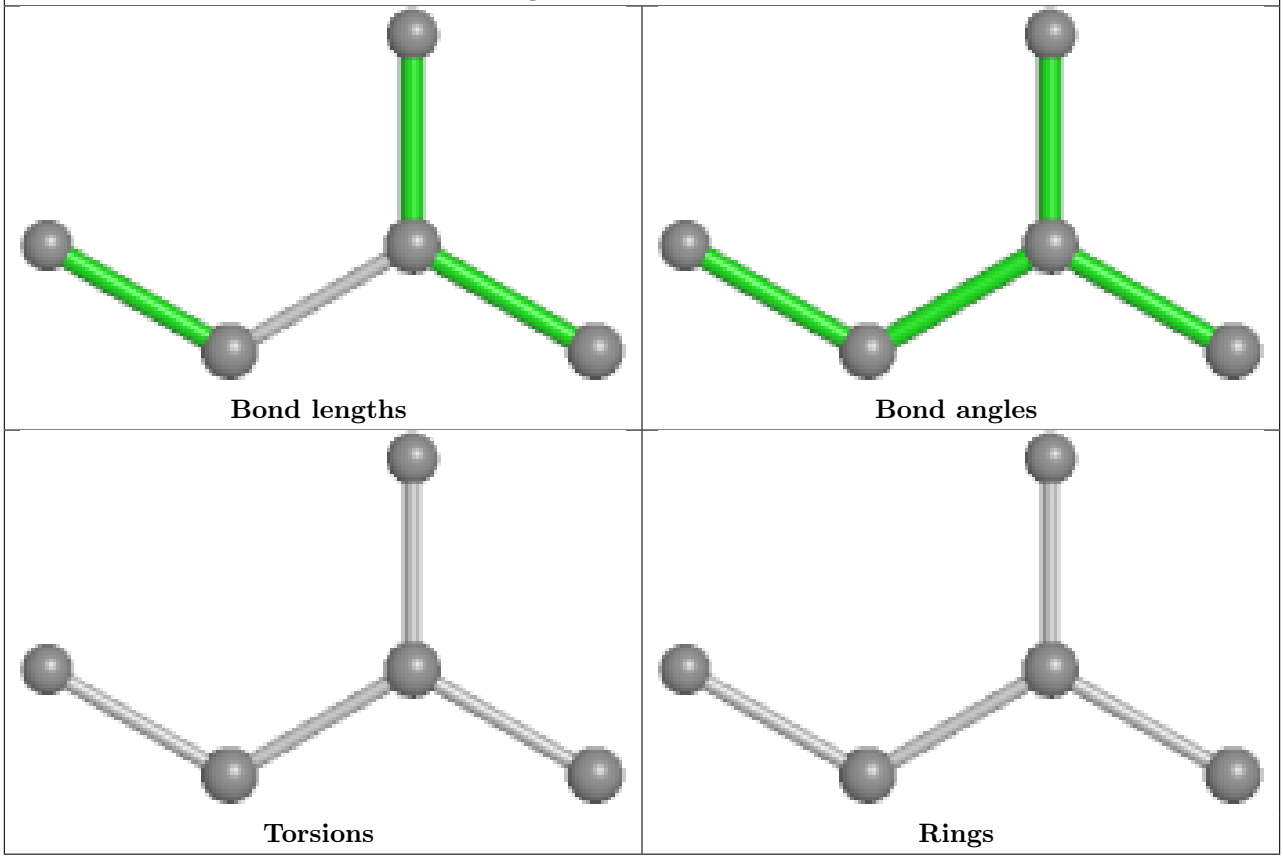


Torsions

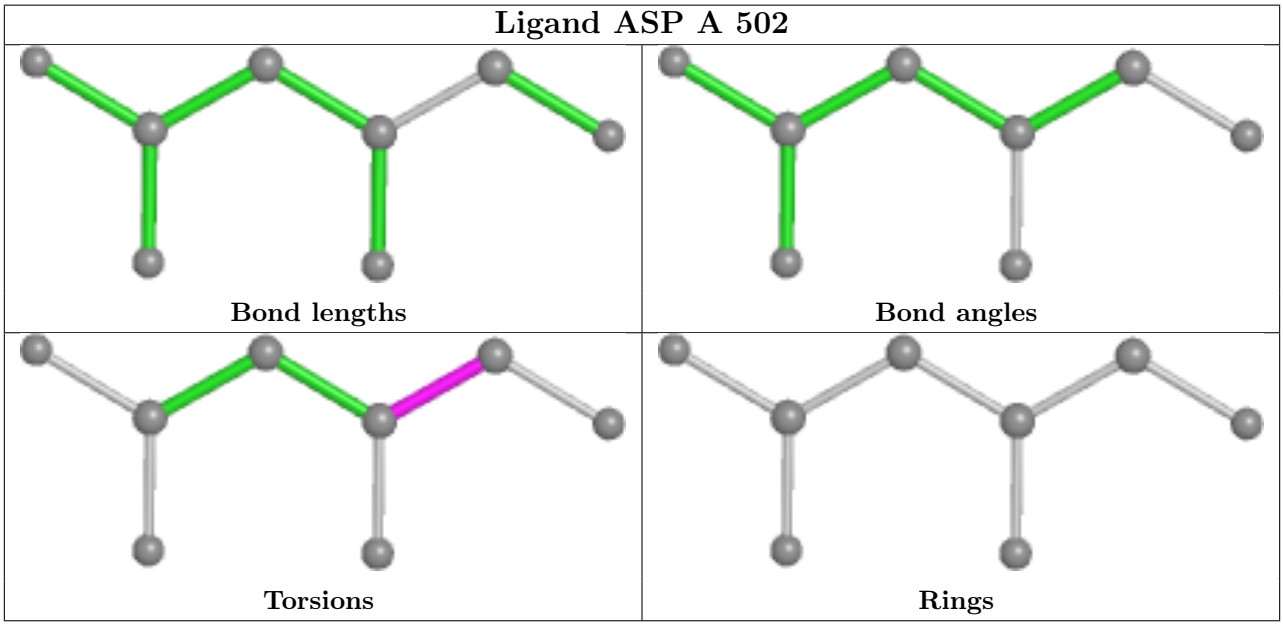


Rings

Ligand ALA A 505



Ligand ASP A 502



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

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, 95^{th} 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	206/467 (44%)	0.44	14 (6%) 17 18	27, 36, 61, 74	0
2	B	206/238 (86%)	0.03	0 100 100	25, 34, 45, 58	0
All	All	412/705 (58%)	0.24	14 (3%) 45 47	25, 35, 55, 74	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	192	THR	4.5
1	A	195	SER	3.8
1	A	133	CYS	3.1
1	A	196	GLN	3.1
1	A	191	SER	3.0

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

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^{th} 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
1	MLY	A	74	11/12	0.89	0.22	45,49,64,64	0
2	MLY	B	79	11/12	0.89	0.16	29,32,52,57	0
2	MLY	B	174	11/12	0.89	0.19	36,43,63,63	0
2	MLY	B	204	11/12	0.90	0.17	34,40,49,53	0
2	MLY	B	188	11/12	0.91	0.17	33,40,57,63	0
1	MLY	A	213	11/12	0.92	0.15	37,42,45,46	0
1	MLY	A	214	11/12	0.92	0.25	40,44,59,65	0
1	MLY	A	38	11/12	0.92	0.24	27,38,55,55	0
1	MLY	A	148	11/12	0.93	0.16	29,31,37,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MLY	A	120	11/12	0.93	0.13	29,33,50,50	0
2	MLY	B	112	11/12	0.93	0.17	33,40,60,62	0
1	MLY	A	67	11/12	0.94	0.12	32,38,48,49	0
2	MLY	B	55	11/12	0.94	0.12	26,30,39,43	0
2	MLY	B	152	11/12	0.94	0.15	29,33,52,52	0
2	MLY	B	212	11/12	0.94	0.11	31,36,58,60	0
1	MLY	A	19	11/12	0.95	0.12	34,38,50,52	0
2	MLY	B	154	11/12	0.95	0.13	29,36,41,42	0
2	MLY	B	147	11/12	0.95	0.13	30,34,41,45	0
2	MLY	B	44	11/12	0.96	0.12	27,32,45,48	0
2	MLY	B	50	11/12	0.96	0.13	26,34,46,48	0

6.3 Carbohydrates (i)

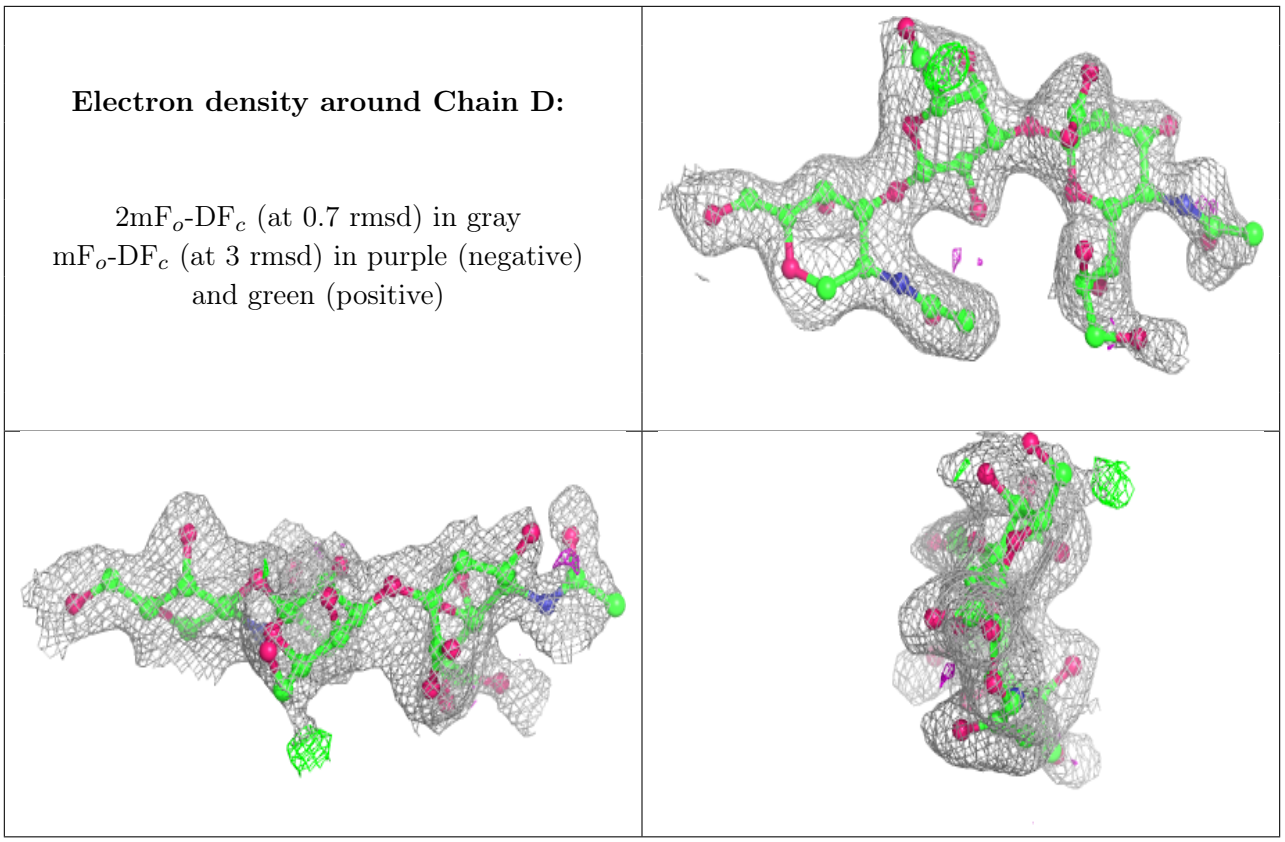
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SIA	D	3	20/21	0.83	0.31	54,62,70,71	0
3	GAL	D	2	11/12	0.86	0.30	46,52,59,61	0
3	A2G	D	1	14/15	0.90	0.15	33,35,41,42	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)



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, 95^{th} 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
10	PEG	A	508	7/7	0.75	0.21	45,47,54,56	0
10	PEG	B	305	7/7	0.81	0.19	47,49,53,54	0
11	GOL	A	509	6/6	0.83	0.24	38,42,47,55	0
10	PEG	B	304	7/7	0.84	0.16	46,48,54,55	0
11	GOL	A	510	6/6	0.86	0.16	53,56,61,65	0
10	PEG	A	507	7/7	0.88	0.17	37,42,45,50	0
10	PEG	B	303	7/7	0.88	0.14	39,45,49,54	0
10	PEG	B	306	7/7	0.89	0.23	42,47,49,50	0
10	PEG	B	307	7/7	0.92	0.16	44,45,48,54	0
4	N7P	A	501	10/11	0.93	0.22	40,42,51,53	0
13	LPD	B	302	8/8	0.93	0.10	35,38,43,49	0
7	ARG	A	504	11/12	0.94	0.10	26,28,33,34	0
9	TRS	A	506	8/8	0.94	0.12	34,35,37,40	0
12	PRO	B	301	7/8	0.95	0.10	30,31,34,35	0

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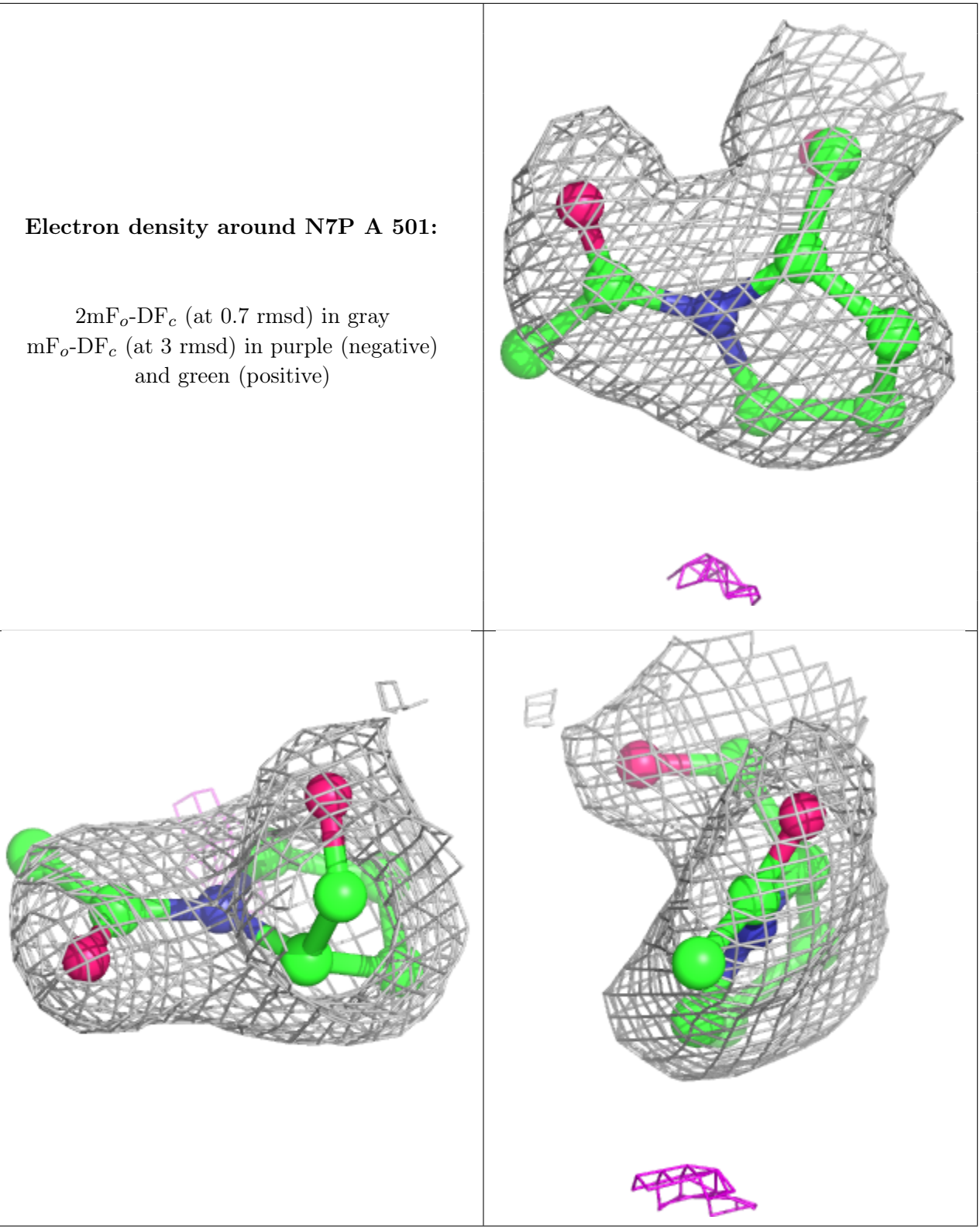
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	THR	A	503	7/8	0.95	0.08	32,33,35,37	0
5	ASP	A	502	8/9	0.96	0.11	34,36,37,38	0
8	ALA	A	505	5/6	0.97	0.13	35,35,37,38	0

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.

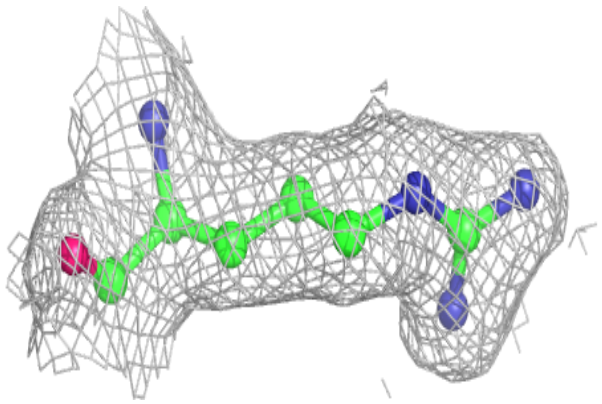
Electron density around N7P A 501:

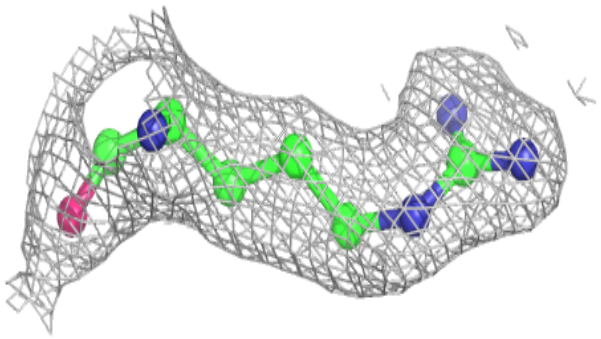
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

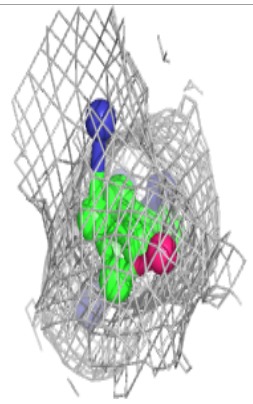


Electron density around ARG A 504:

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

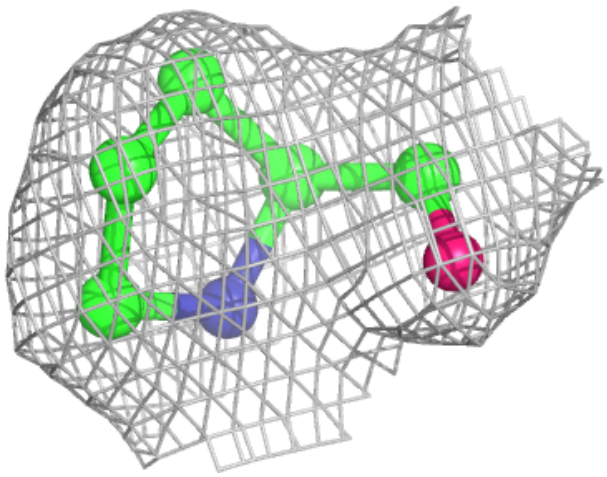


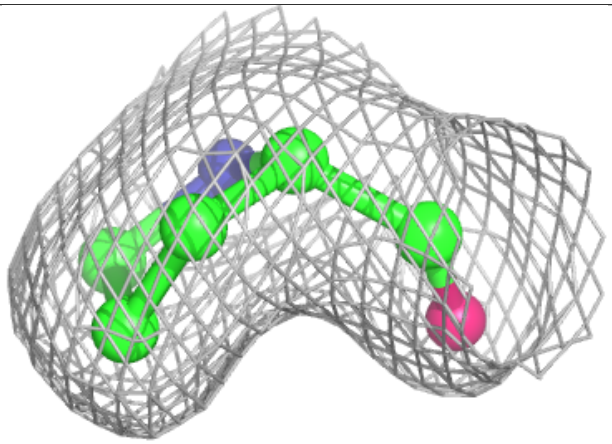


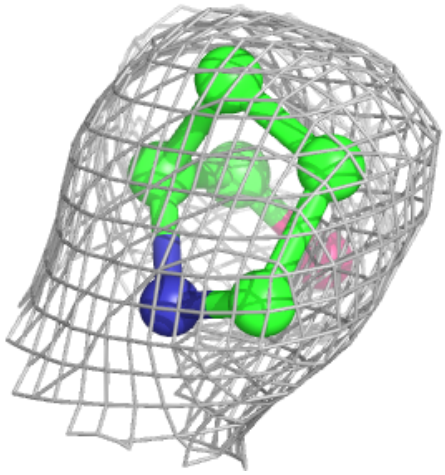


Electron density around PRO B 301:

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

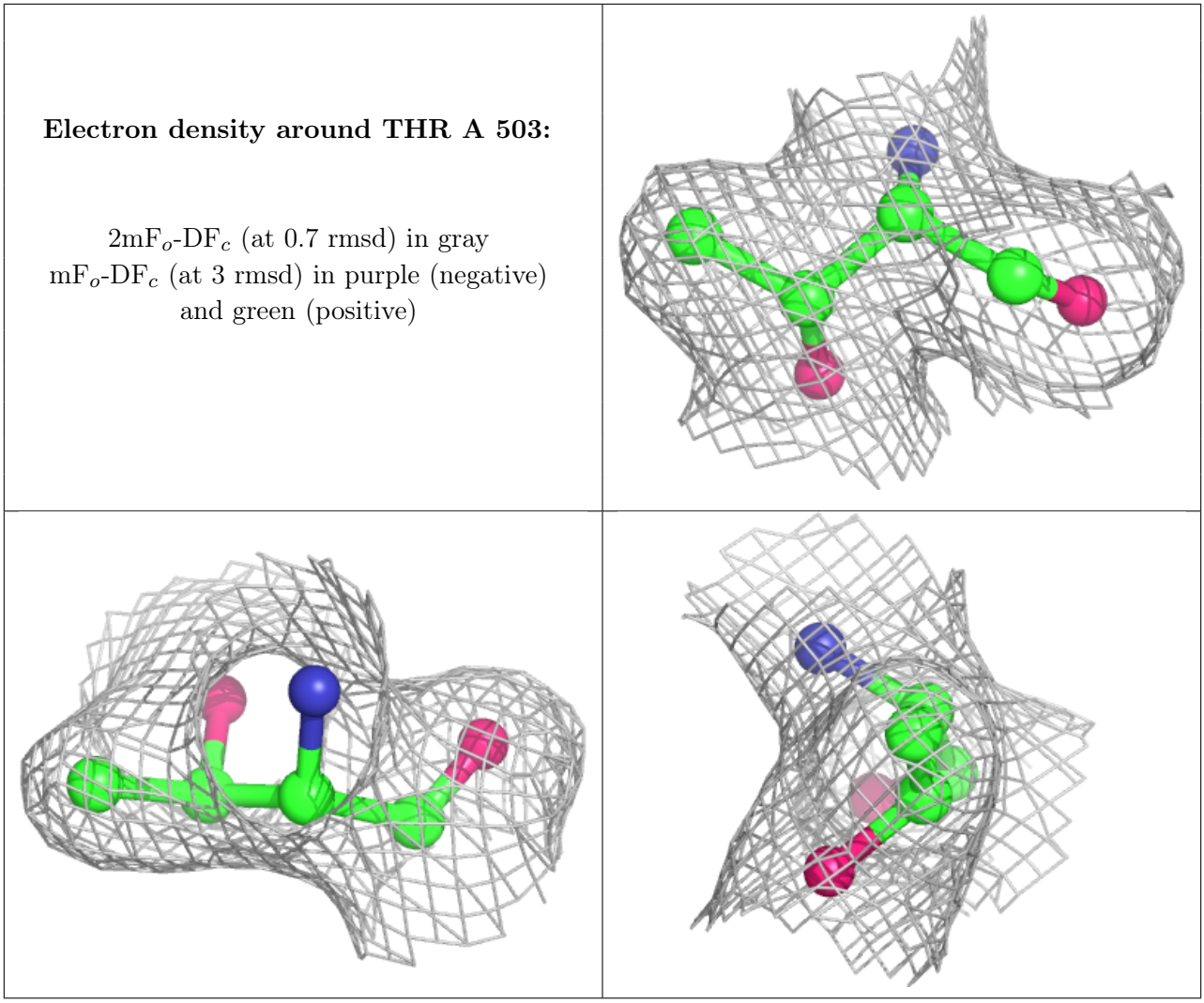






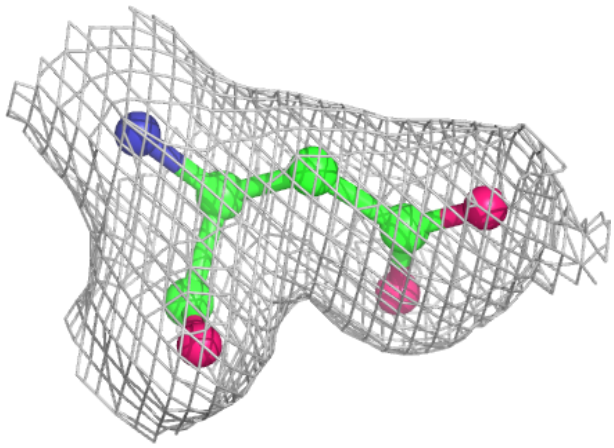
Electron density around THR A 503:

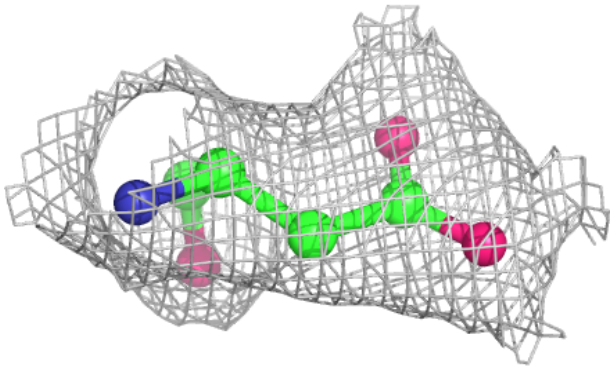
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

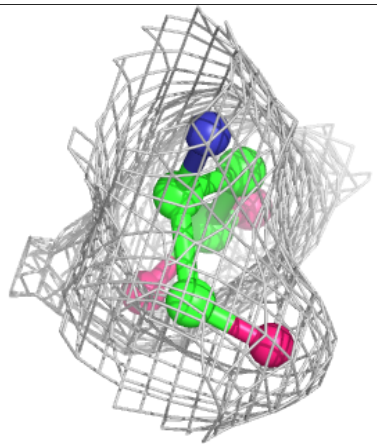


Electron density around ASP A 502:

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

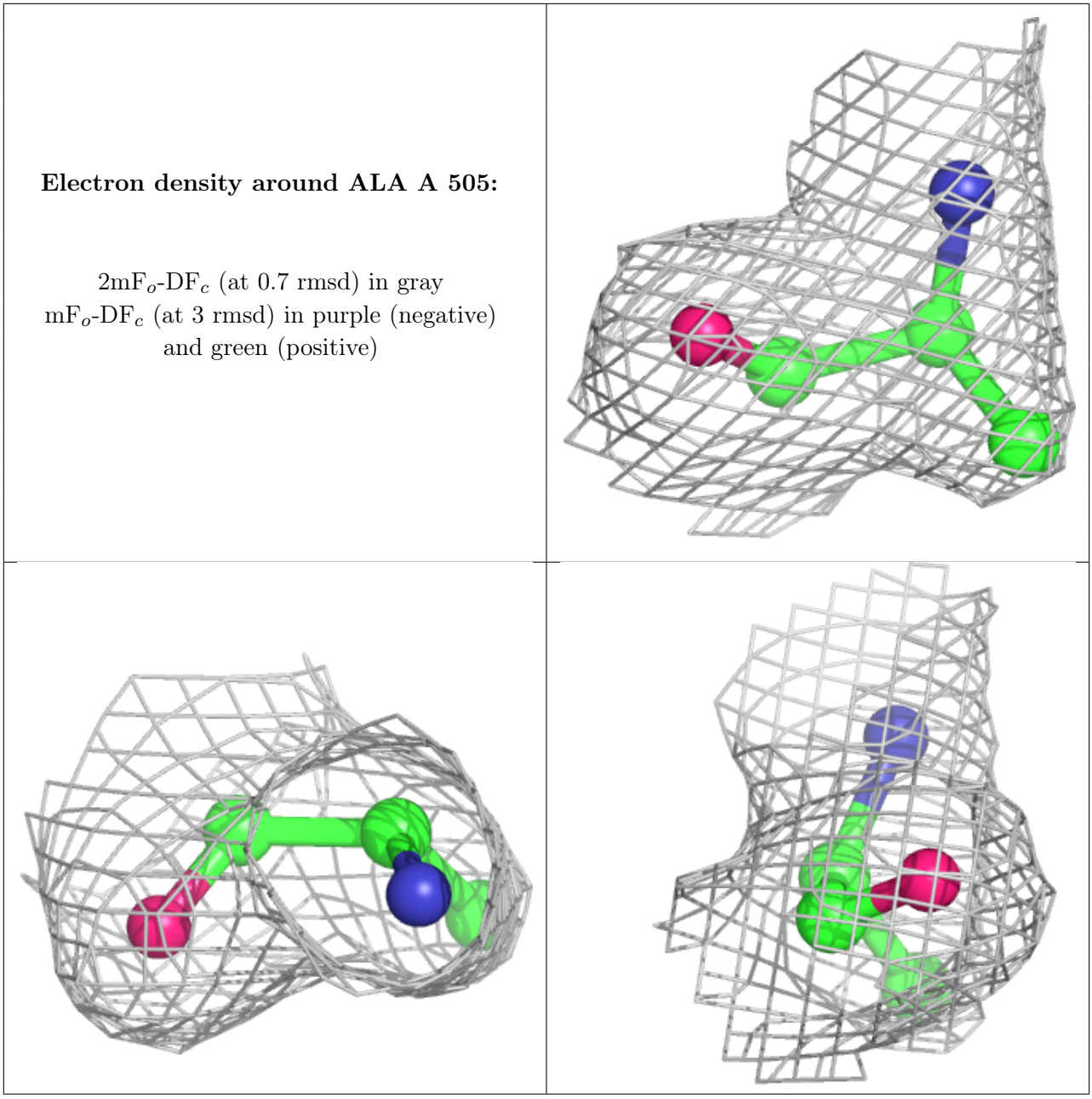






Electron density around ALA A 505:

$2mF_o$-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.