



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:58 PM UTC

PDB ID : 8HRH / pdb_00008hrh
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

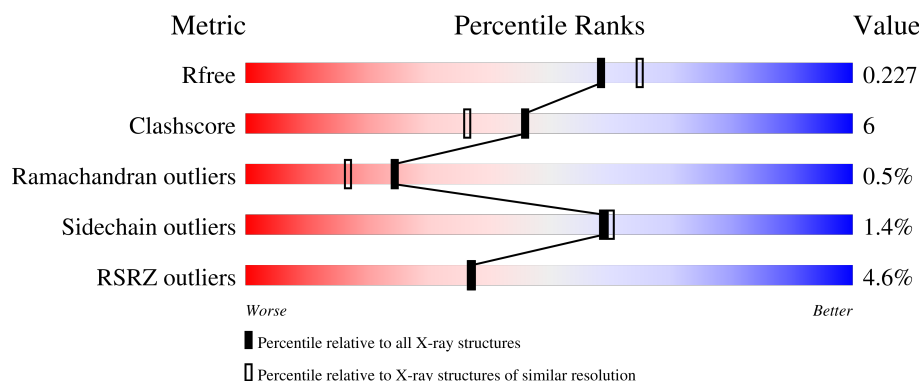
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (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 $\leq 5\%$. 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	467	 3% 38% 7% 54%
2	B	238	 % 79% 11% 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.

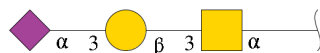
- Molecule 1 is a protein called Heavy chain of SN-131/1B2 antibody Fab.

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

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

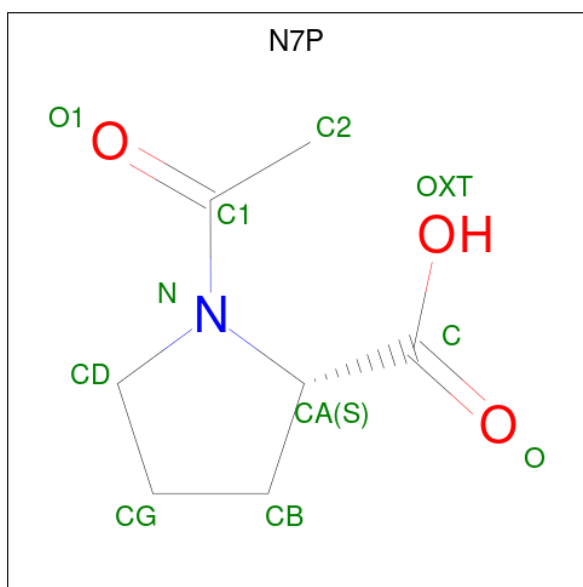
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1716	1082	287	341	6			

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



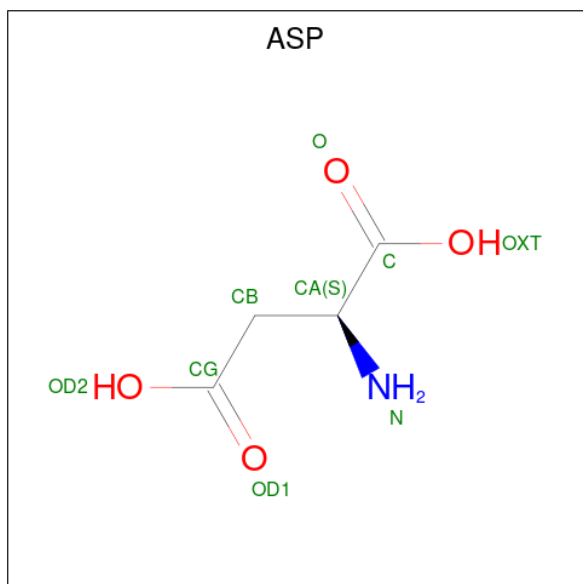
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			45	25	2	18			

- Molecule 4 is 1-ACETYL-L-PROLINE (CCD ID: N7P) (formula: C₇H₁₁NO₃) (labeled as "Ligand of Interest" by depositor).



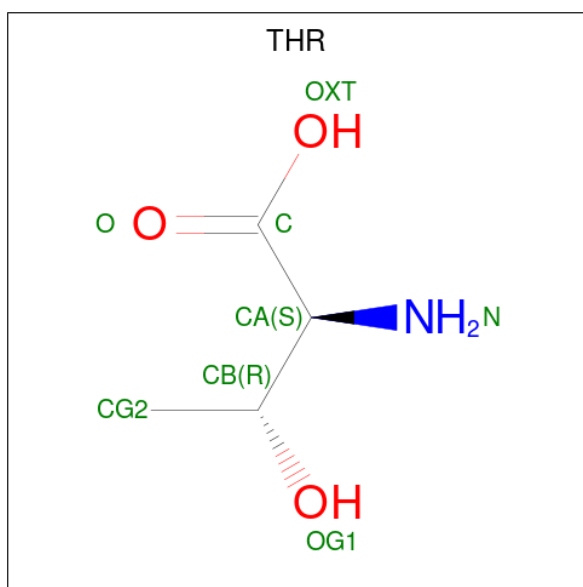
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	7	1	2		

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



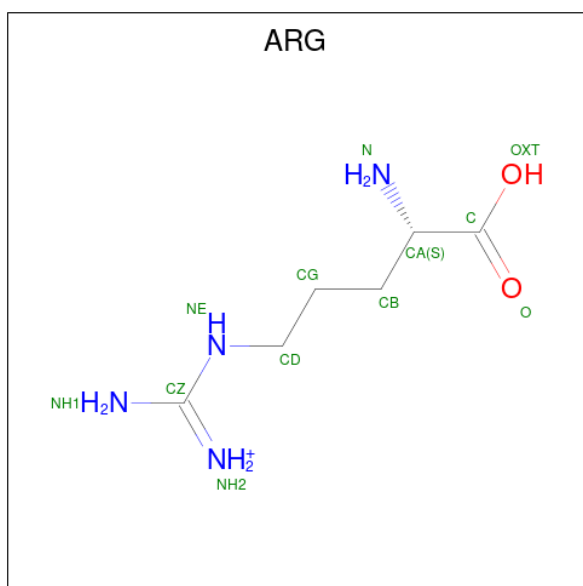
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		

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



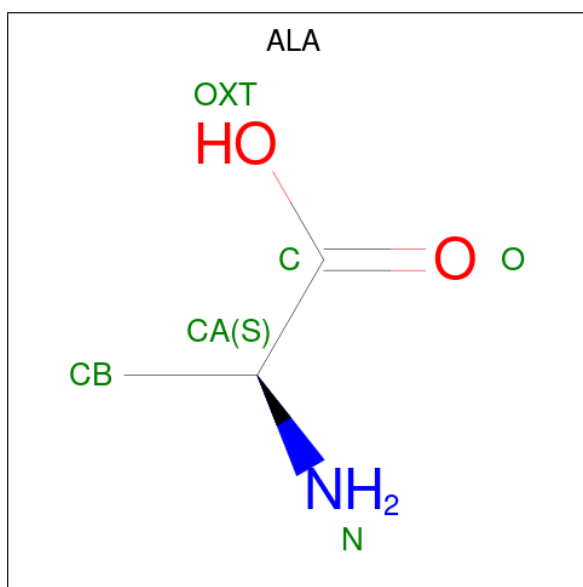
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 7 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



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

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



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

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

- Molecule 10 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



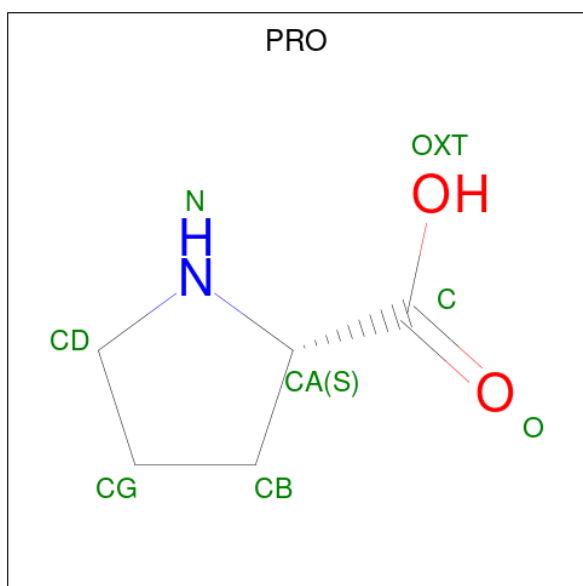
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			7	4	3		
10	A	1	Total	C	O	0	0
			7	4	3		
10	B	1	Total	C	O	0	0
			7	4	3		
10	B	1	Total	C	O	0	0
			7	4	3		
10	B	1	Total	C	O	0	0
			7	4	3		
10	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



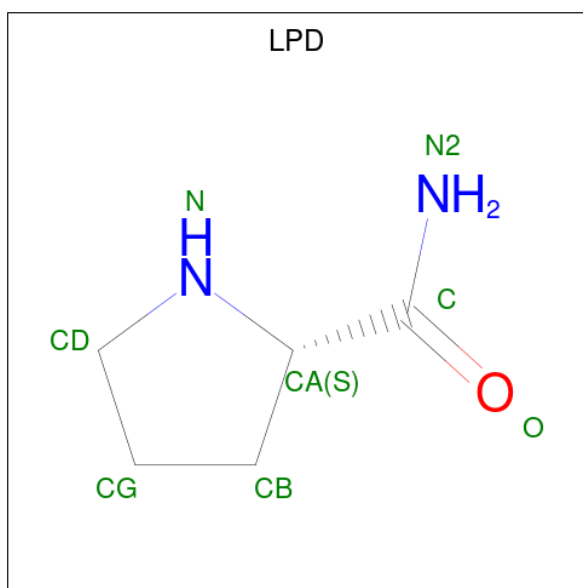
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			6	3	3		
11	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 12 is PROLINE (CCD ID: 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	0	0
			7	5	1	1		

- Molecule 13 is L-PROLINAMIDE (CCD ID: LPD) (formula: $C_5H_{10}N_2O$).



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

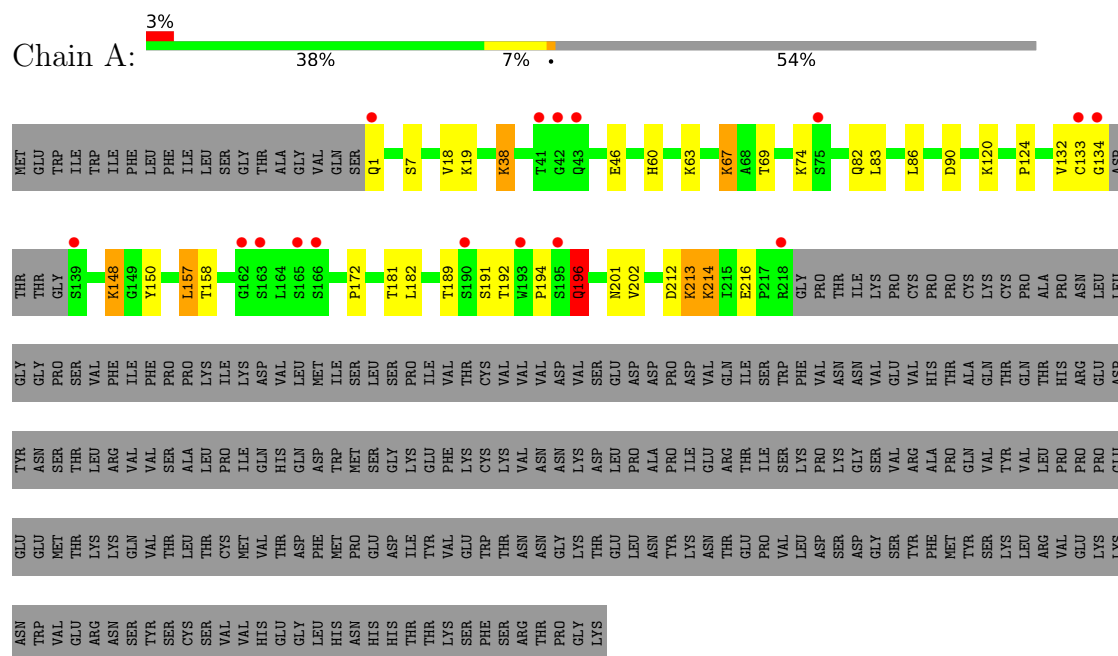
- Molecule 14 is water.

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

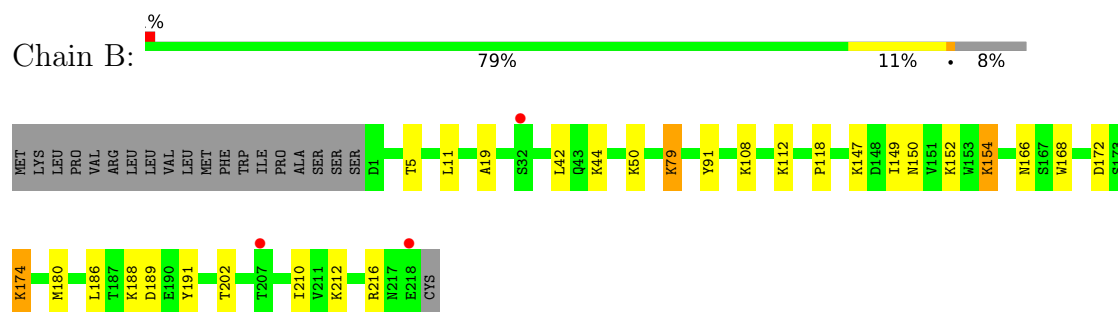
3 Residue-property plots

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



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



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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.16-3549	Depositor
R, R_{free}	0.192 , 0.227 0.195 , 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)	0.36 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MLY, PEG, GAL, LPD, N7P, A2G, TRS, SIA

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	0.21	0/1562	0.45	0/2139
2	B	0.23	0/1624	0.44	0/2218
All	All	0.22	0/3186	0.44	0/4357

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1612	0	1585	25	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
9	A	8	0	12	1	0
10	A	14	0	20	2	0
10	B	35	0	50	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	40	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.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:LYS:HB2	10:B:306:PEG:H32	1.66	0.77
11:A:510:GOL:O1	11:A:510:GOL:O3	2.04	0.73
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
1:A:172:PRO:HA	10:A:507:PEG:H32	1.87	0.56
1:A:214:MLY:HE2	1:A:216:GLU:OE2	2.08	0.54
1:A:148:MLY:HH12	14:A:686:HOH:O	2.10	0.51
1:A:212:ASP:O	1:A:213:MLY:HD3	2.09	0.51
1:A:69:THR:HG23	14:A:607:HOH:O	2.10	0.51
1:A:1:GLN:OE1	1:A:1:GLN:N	2.39	0.50
1:A:189:THR:HG22	1:A:191:SER:H	1.76	0.50
1:A:38:MLY:HH23	1:A:90:ASP:HA	1.93	0.49
1:A:18:VAL:HG12	1:A:86:LEU:HD11	1.94	0.49
1:A:132:VAL:O	1:A:134:GLY:N	2.46	0.48
1:A:60:HIS:ND1	11:A:509:GOL:H11	2.28	0.48
2:B:174:MLY:HD3	10:B:307:PEG:H42	1.96	0.48
2:B:11:LEU:HD21	2:B:19:ALA:HB1	1.96	0.47
2:B:154:MLY:HD2	2:B:154:MLY:HH22	1.58	0.47
2:B:191:TYR:CZ	2:B:216:ARG:HD3	2.50	0.47
1:A:192:THR:O	1:A:196:GLN:HB2	2.16	0.46
1:A:148:MLY:HH23	1:A:181:THR:OG1	2.16	0.45
1:A:82:GLN:HG3	14:A:601:HOH:O	2.17	0.44
2:B:150:ASN:HB2	2:B:202:THR:OG1	2.17	0.44
2:B:118:PRO:HG2	2:B:210:ILE:HD12	1.98	0.43
1:A:7:SER:HB3	11:A:510:GOL:H12	2.01	0.43
1:A:158:THR:HG23	1:A:201:ASN:OD1	2.19	0.43
2:B:42:LEU:HD13	2:B:91:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:ASN:HB3	2:B:180:MET:HE2	2.01	0.43
1:A:148:MLY:HH22	1:A:148:MLY:HD3	1.79	0.43
1:A:158:THR:HG22	1:A:201:ASN:HB2	2.01	0.42
9:A:506:TRS:N	10:A:507:PEG:H31	2.35	0.42
1:A:60:HIS:HB3	11:A:509:GOL:H12	2.01	0.41
1:A:124:PRO:HB3	1:A:150:TYR:HB3	2.01	0.41
2:B:149:ILE:HG22	2:B:168:TRP:CZ3	2.55	0.41
1:A:83:LEU:N	14:A:601:HOH:O	2.53	0.41
1:A:67:MLY:HH23	1:A:67:MLY:HD2	1.75	0.41
1:A:46:GLU:OE2	1:A:63:LYS:HD3	2.20	0.41
1:A:194:PRO:C	1:A:196:GLN:H	2.28	0.41
2:B:79:MLY:HG2	14:B:420:HOH:O	2.21	0.41

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%)	12	5
2	B	204/238 (86%)	198 (97%)	6 (3%)	0	100	100
All	All	406/705 (58%)	392 (97%)	12 (3%)	2 (0%)	24	17

All (2) Ramachandran outliers are listed below:

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

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	170/405 (42%)	167 (98%)	3 (2%)	51	51
2	B	182/201 (90%)	180 (99%)	2 (1%)	65	68
All	All	352/606 (58%)	347 (99%)	5 (1%)	59	60

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

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	195	ASN
2	B	215	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
2	MLY	B	55	2	9,10,11	0.94	0	6,11,13	0.61	0
2	MLY	B	112	2	9,10,11	1.00	1 (11%)	6,11,13	0.94	0
1	MLY	A	213	1	9,10,11	1.04	1 (11%)	6,11,13	0.70	0
2	MLY	B	152	2	9,10,11	0.95	1 (11%)	6,11,13	0.73	0
2	MLY	B	79	2	9,10,11	0.97	1 (11%)	6,11,13	0.65	0
2	MLY	B	44	2	9,10,11	0.95	1 (11%)	6,11,13	1.11	1 (16%)
1	MLY	A	148	1	9,10,11	1.06	1 (11%)	6,11,13	0.88	0
2	MLY	B	174	2	9,10,11	1.02	1 (11%)	6,11,13	0.65	0
2	MLY	B	50	2	9,10,11	0.93	1 (11%)	6,11,13	0.93	0
1	MLY	A	38	1	9,10,11	1.02	1 (11%)	6,11,13	1.05	0
1	MLY	A	67	1	9,10,11	1.00	1 (11%)	6,11,13	0.79	0
1	MLY	A	214	1	9,10,11	1.06	1 (11%)	6,11,13	0.61	0
2	MLY	B	212	2	9,10,11	0.95	1 (11%)	6,11,13	0.78	0
2	MLY	B	147	2	9,10,11	0.99	1 (11%)	6,11,13	0.99	1 (16%)
1	MLY	A	120	1	9,10,11	1.01	1 (11%)	6,11,13	0.74	0
1	MLY	A	19	1	9,10,11	1.00	1 (11%)	6,11,13	0.67	0
2	MLY	B	204	2	9,10,11	0.97	0	6,11,13	0.54	0
2	MLY	B	188	2	9,10,11	0.97	1 (11%)	6,11,13	0.85	0
1	MLY	A	74	1	9,10,11	0.98	1 (11%)	6,11,13	0.84	0
2	MLY	B	154	2	9,10,11	1.02	1 (11%)	6,11,13	0.65	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
2	MLY	B	55	2	-	2/8/9/11	-
2	MLY	B	112	2	-	2/8/9/11	-
1	MLY	A	213	1	-	5/8/9/11	-
2	MLY	B	152	2	-	2/8/9/11	-
2	MLY	B	79	2	-	5/8/9/11	-
2	MLY	B	44	2	-	2/8/9/11	-
1	MLY	A	148	1	-	4/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLY	B	174	2	-	3/8/9/11	-
2	MLY	B	50	2	-	2/8/9/11	-
1	MLY	A	38	1	-	2/8/9/11	-
1	MLY	A	67	1	-	1/8/9/11	-
1	MLY	A	214	1	-	0/8/9/11	-
2	MLY	B	212	2	-	0/8/9/11	-
2	MLY	B	147	2	-	0/8/9/11	-
1	MLY	A	120	1	-	1/8/9/11	-
1	MLY	A	19	1	-	1/8/9/11	-
2	MLY	B	204	2	-	2/8/9/11	-
2	MLY	B	188	2	-	4/8/9/11	-
1	MLY	A	74	1	-	2/8/9/11	-
2	MLY	B	154	2	-	4/8/9/11	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	MLY	CA-N	-2.45	1.41	1.48
2	B	112	MLY	CA-N	-2.45	1.41	1.48
1	A	214	MLY	CA-N	-2.43	1.41	1.48
2	B	154	MLY	CA-N	-2.37	1.41	1.48
1	A	213	MLY	CA-N	-2.34	1.41	1.48
2	B	174	MLY	CA-N	-2.28	1.41	1.48
2	B	188	MLY	CA-N	-2.26	1.41	1.48
1	A	19	MLY	CA-N	-2.23	1.41	1.48
1	A	38	MLY	CA-N	-2.23	1.41	1.48
1	A	120	MLY	CA-N	-2.20	1.41	1.48
1	A	67	MLY	CA-N	-2.20	1.41	1.48
1	A	74	MLY	CA-N	-2.19	1.41	1.48
2	B	212	MLY	CA-N	-2.16	1.42	1.48
2	B	50	MLY	CA-N	-2.15	1.42	1.48
2	B	79	MLY	CA-N	-2.13	1.42	1.48
2	B	152	MLY	CA-N	-2.10	1.42	1.48
2	B	147	MLY	CA-N	-2.09	1.42	1.48
2	B	44	MLY	CA-N	-2.09	1.42	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	44	MLY	CD-CE-NZ	-2.14	108.18	113.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	147	MLY	CD-CE-NZ	-2.06	108.38	113.71

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	38	MLY	N-CA-CB-CG
1	A	38	MLY	C-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
2	B	152	MLY	O-C-CA-CB
2	B	204	MLY	C-CA-CB-CG
1	A	148	MLY	CD-CE-NZ-CH2
1	A	213	MLY	CD-CE-NZ-CH1
2	B	44	MLY	CD-CE-NZ-CH1
2	B	44	MLY	CD-CE-NZ-CH2
2	B	174	MLY	CD-CE-NZ-CH2
2	B	188	MLY	CD-CE-NZ-CH1
2	B	154	MLY	CG-CD-CE-NZ
1	A	19	MLY	CG-CD-CE-NZ
1	A	148	MLY	CD-CE-NZ-CH1
1	A	213	MLY	CD-CE-NZ-CH2
2	B	174	MLY	CD-CE-NZ-CH1
2	B	188	MLY	CD-CE-NZ-CH2
1	A	74	MLY	CG-CD-CE-NZ
1	A	148	MLY	CG-CD-CE-NZ
1	A	213	MLY	CG-CD-CE-NZ
2	B	79	MLY	CG-CD-CE-NZ
2	B	154	MLY	CD-CE-NZ-CH2
2	B	79	MLY	CE-CD-CG-CB
2	B	204	MLY	CG-CD-CE-NZ
2	B	55	MLY	CD-CE-NZ-CH2
2	B	79	MLY	CD-CE-NZ-CH2
2	B	174	MLY	CE-CD-CG-CB
2	B	154	MLY	C-CA-CB-CG
2	B	188	MLY	C-CA-CB-CG
2	B	79	MLY	CD-CE-NZ-CH1
2	B	188	MLY	CE-CD-CG-CB
2	B	50	MLY	N-CA-CB-CG
2	B	112	MLY	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	67	MLY	CD-CE-NZ-CH2
2	B	55	MLY	CG-CD-CE-NZ
1	A	148	MLY	CA-CB-CG-CD
1	A	74	MLY	CD-CE-NZ-CH2
2	B	79	MLY	CA-CB-CG-CD
1	A	120	MLY	CE-CD-CG-CB
2	B	152	MLY	C-CA-CB-CG
2	B	154	MLY	CA-CB-CG-CD

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
2	B	79	MLY	1	0
1	A	148	MLY	3	0
2	B	174	MLY	2	0
1	A	38	MLY	1	0
1	A	67	MLY	1	0
1	A	214	MLY	1	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	0.26	0	17,19,21	1.00	1 (5%)
3	GAL	D	2	3	11,11,12	0.22	0	15,15,17	0.60	0
3	SIA	D	3	3	20,20,21	0.51	0	21,28,31	1.12	3 (14%)

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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	A2G	C1-O5-C5	2.86	116.02	112.19
3	D	3	SIA	O1B-C1-C2	2.80	119.99	112.71
3	D	3	SIA	O6-C2-C1	2.57	112.58	107.72
3	D	3	SIA	O1A-C1-C2	-2.31	117.87	122.85

There are no chirality outliers.

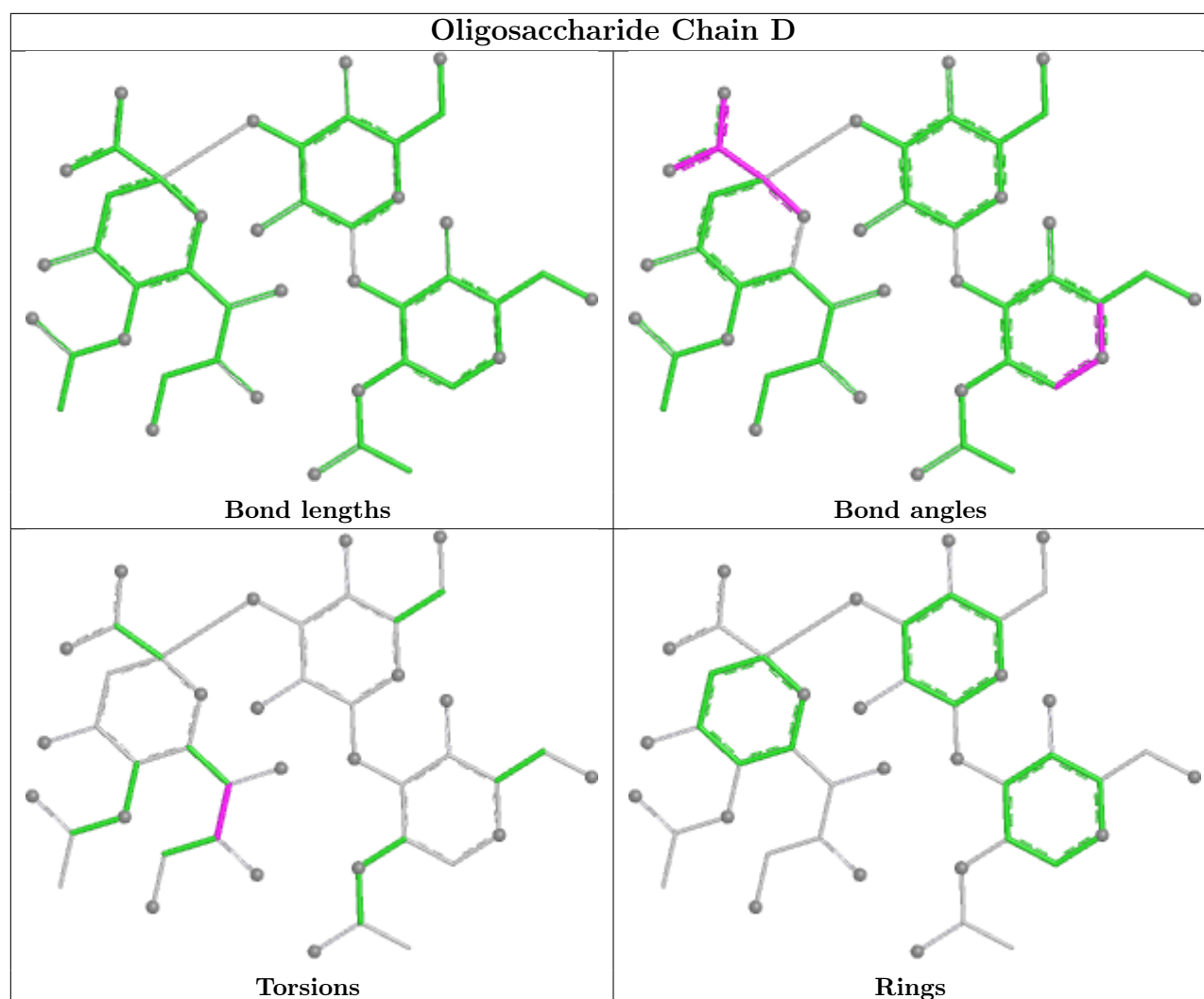
All (3) torsion outliers are listed below:

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.



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	$\# Z > 2$
13	LPD	B	302	-	8,8,8	1.55	1 (12%)	10,10,10	1.21	0
10	PEG	B	306	-	6,6,6	0.49	0	5,5,5	0.23	0
8	ALA	A	505	12	3,4,5	0.70	0	2,4,6	0.83	0
7	ARG	A	504	12	9,10,11	0.52	0	5,11,13	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	TRS	A	506	-	7,7,7	0.56	0	9,9,9	0.40	0
10	PEG	B	304	-	6,6,6	0.51	0	5,5,5	0.35	0
6	THR	A	503	3	5,6,7	0.57	0	5,7,9	0.68	0
10	PEG	A	507	-	6,6,6	0.50	0	5,5,5	0.35	0
10	PEG	B	307	-	6,6,6	0.52	0	5,5,5	0.27	0
11	GOL	A	509	-	5,5,5	1.15	0	5,5,5	0.86	0
10	PEG	B	305	-	6,6,6	0.50	0	5,5,5	0.18	0
4	N7P	A	501	5	9,10,11	1.40	1 (11%)	9,13,15	1.85	3 (33%)
12	PRO	B	301	8,7	6,7,8	0.62	0	7,8,10	1.00	0
10	PEG	A	508	-	6,6,6	0.48	0	5,5,5	0.34	0
5	ASP	A	502	4	6,7,8	1.00	0	4,8,10	0.82	0
10	PEG	B	303	-	6,6,6	0.50	0	5,5,5	0.34	0
11	GOL	A	510	-	5,5,5	0.84	0	5,5,5	0.84	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
13	LPD	B	302	-	-	2/4/11/11	0/1/1/1
10	PEG	B	306	-	-	2/4/4/4	-
8	ALA	A	505	12	-	1/1/2/4	-
7	ARG	A	504	12	-	1/8/9/11	-
9	TRS	A	506	-	-	0/9/9/9	-
10	PEG	B	304	-	-	1/4/4/4	-
6	THR	A	503	3	-	1/5/6/8	-
10	PEG	A	507	-	-	1/4/4/4	-
10	PEG	B	307	-	-	1/4/4/4	-
11	GOL	A	509	-	-	1/4/4/4	-
10	PEG	B	305	-	-	1/4/4/4	-
4	N7P	A	501	5	-	0/4/16/18	0/1/1/1
12	PRO	B	301	8,7	-	0/0/9/11	0/1/1/1
10	PEG	A	508	-	-	1/4/4/4	-
5	ASP	A	502	4	-	1/5/6/8	-
10	PEG	B	303	-	-	1/4/4/4	-
11	GOL	A	510	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	302	LPD	C-N2	3.87	1.42	1.32
4	A	501	N7P	CA-N	-3.33	1.45	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	N7P	C2-C1-N	3.77	122.06	117.99
4	A	501	N7P	CA-N-C1	3.04	126.93	120.82
4	A	501	N7P	CG-CD-N	2.12	106.88	103.24

There are no chirality outliers.

All (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
8	A	505	ALA	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
10	B	303	PEG	O2-C3-C4-O4
10	B	307	PEG	O1-C1-C2-O2
11	A	510	GOL	O1-C1-C2-C3
10	B	304	PEG	O2-C3-C4-O4
10	B	306	PEG	O1-C1-C2-O2
10	A	508	PEG	O2-C3-C4-O4
10	B	305	PEG	O1-C1-C2-O2
11	A	510	GOL	O1-C1-C2-O2
11	A	509	GOL	O1-C1-C2-O2
10	B	306	PEG	C1-C2-O2-C3
6	A	503	THR	O-C-CA-CB

There are no ring outliers.

7 monomers are involved in 9 short contacts:

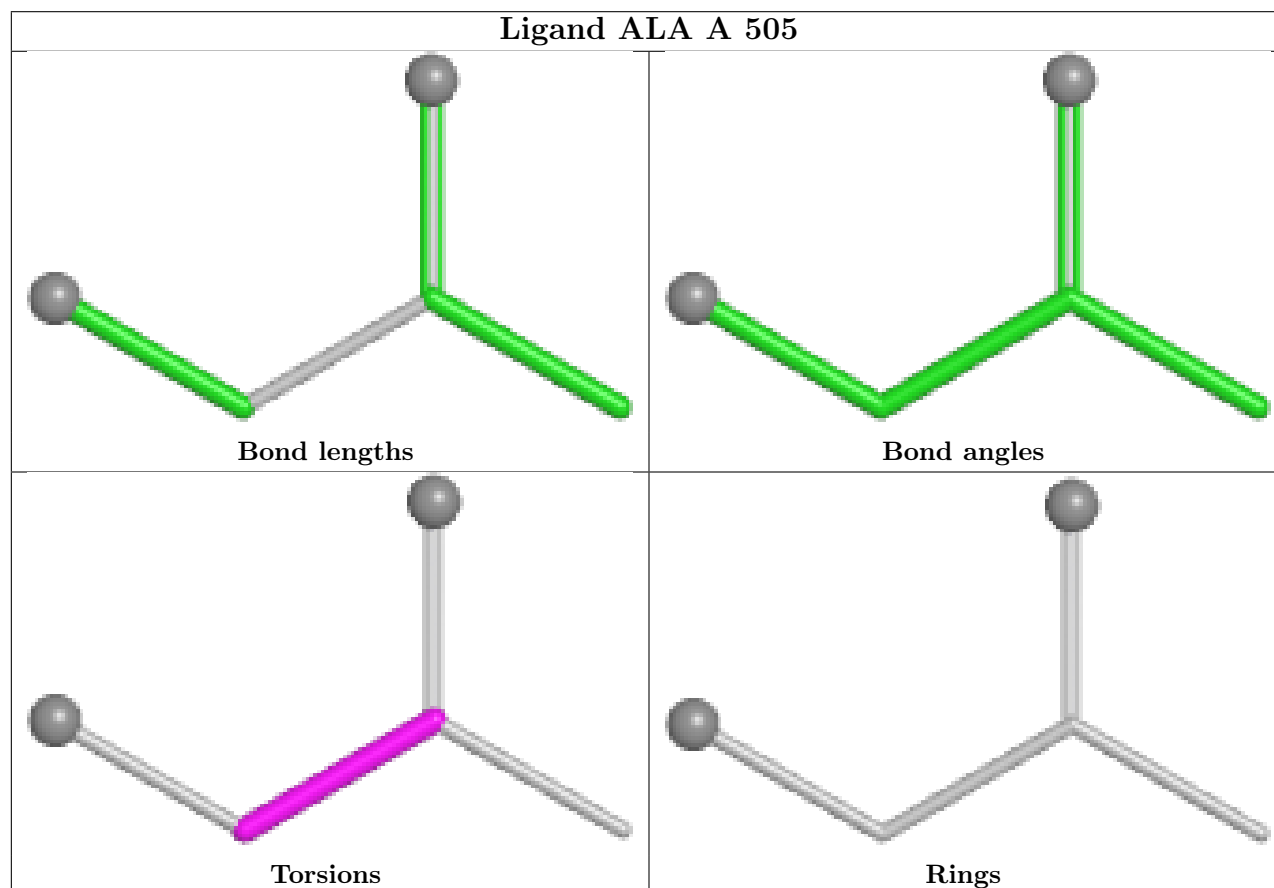
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	306	PEG	1	0
9	A	506	TRS	1	0
10	A	507	PEG	2	0
10	B	307	PEG	1	0
11	A	509	GOL	2	0
10	B	305	PEG	1	0

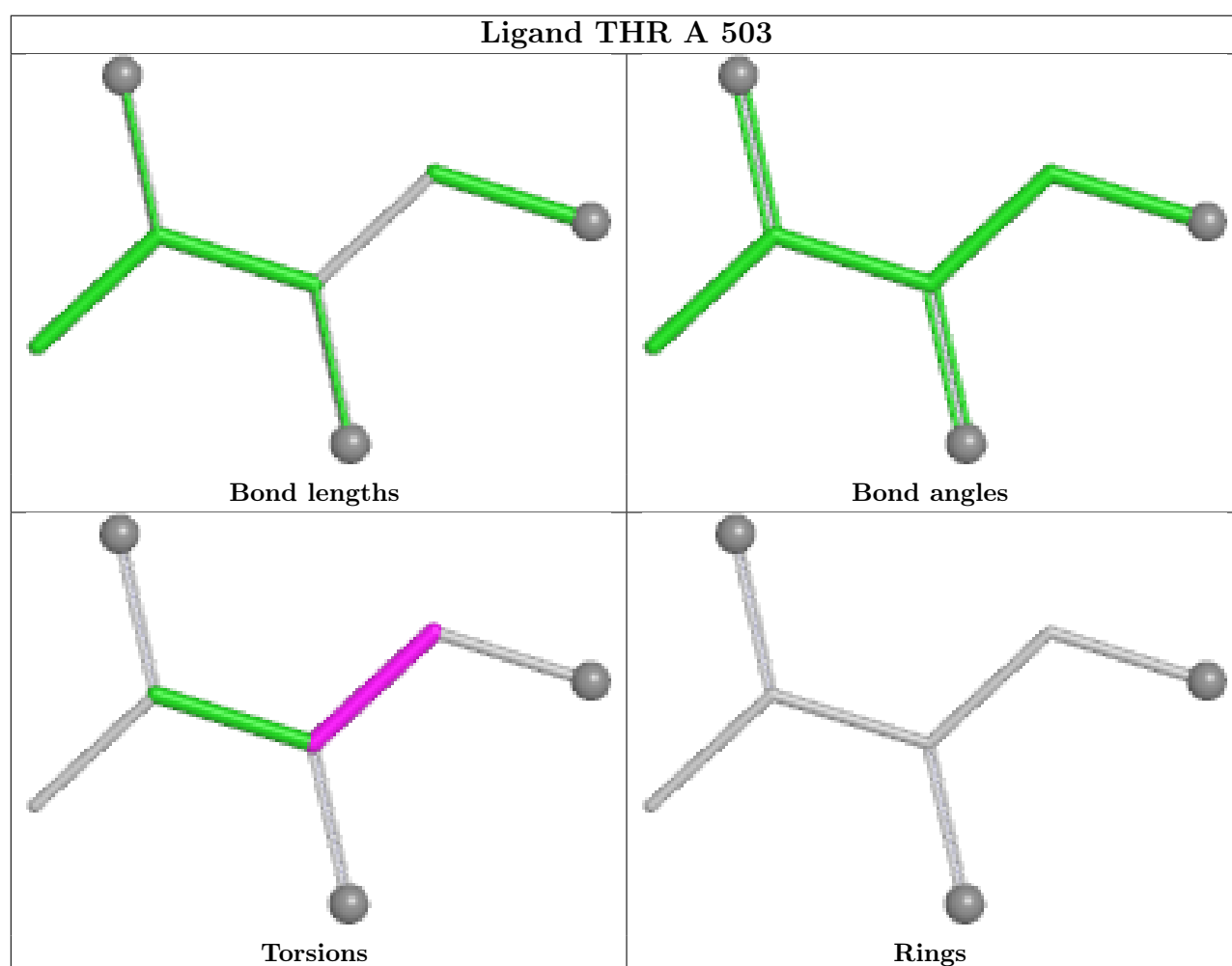
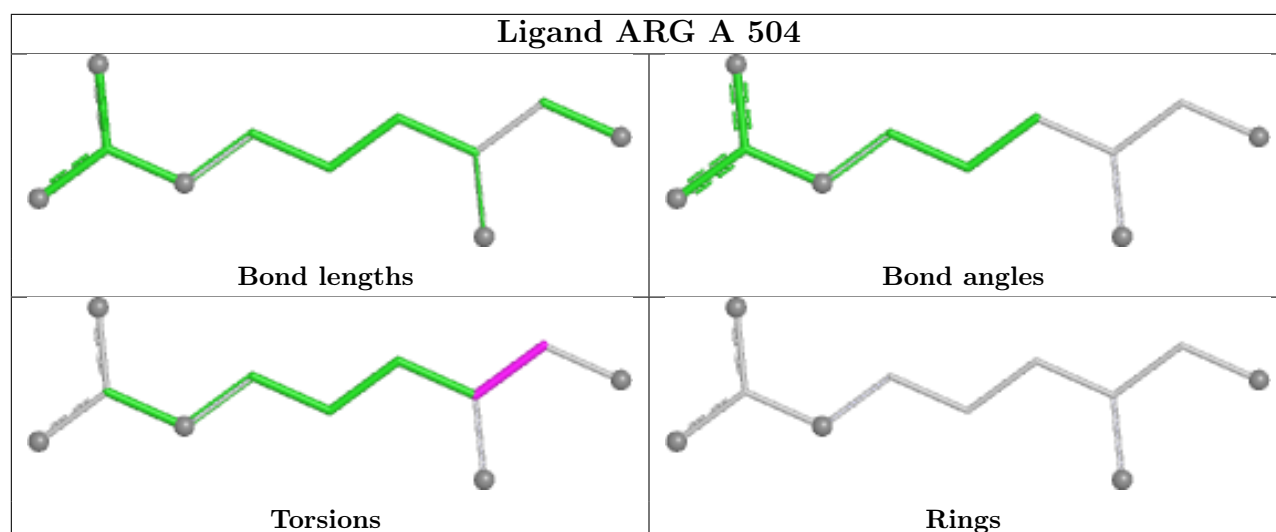
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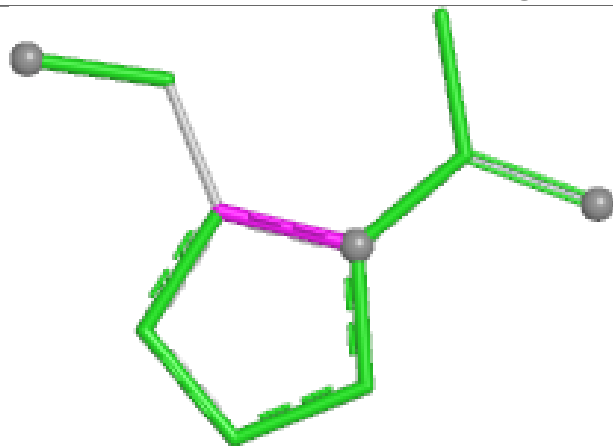
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	510	GOL	2	0

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.





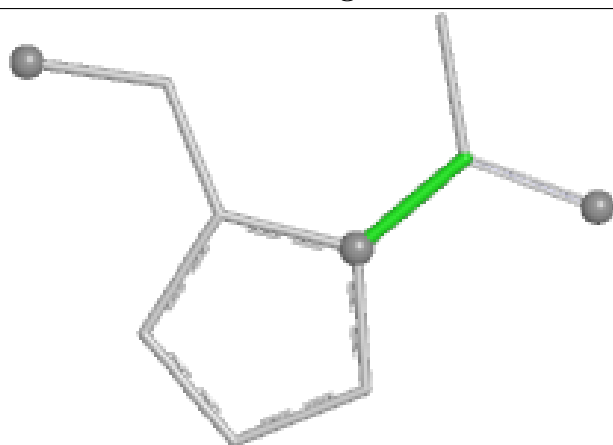
Ligand N7P A 501



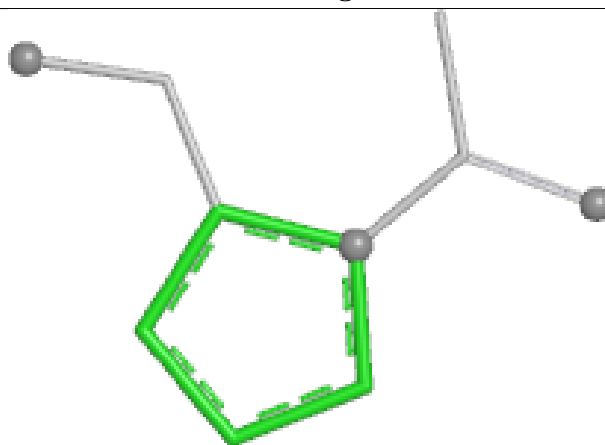
Bond lengths



Bond angles

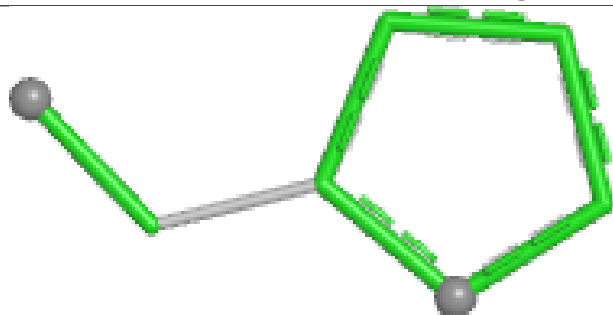


Torsions

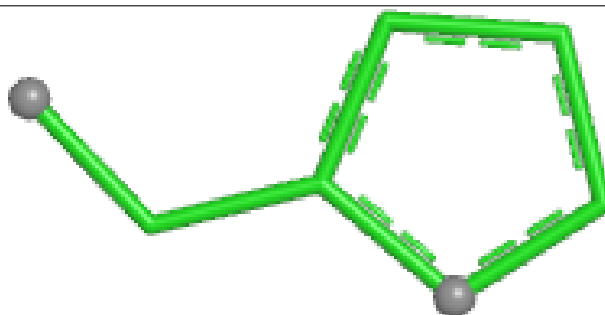


Rings

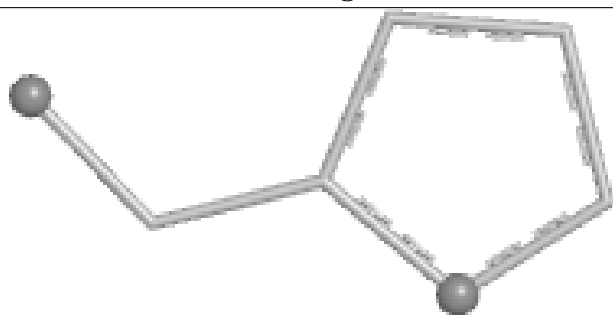
Ligand PRO B 301



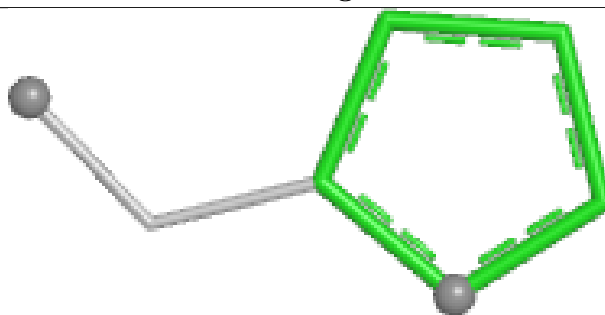
Bond lengths



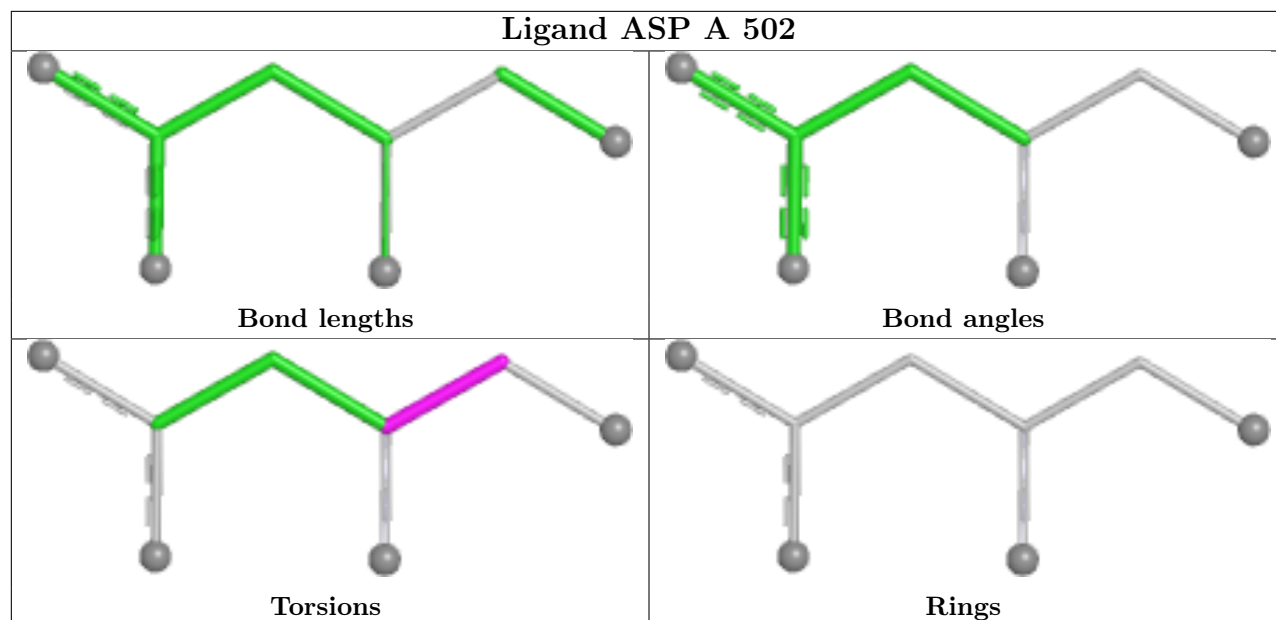
Bond angles



Torsions



Rings



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	206/467 (44%)	0.39	16 (7%) 19 19	27, 36, 61, 74	0
2	B	206/238 (86%)	0.04	3 (1%) 72 74	25, 34, 45, 58	0
All	All	412/705 (58%)	0.21	19 (4%) 37 37	25, 35, 55, 74	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	GLY	4.7
1	A	41	THR	4.4
1	A	163	SER	3.3
1	A	1	GLN	2.9
2	B	207	THR	2.8
1	A	42	GLY	2.7
1	A	218	ARG	2.6
1	A	139	SER	2.5
1	A	195	SER	2.5
1	A	162	GLY	2.5
1	A	193	TRP	2.5
1	A	190	SER	2.4
2	B	218	GLU	2.4
1	A	133	CYS	2.2
1	A	165	SER	2.2
2	B	32	SER	2.2
1	A	43	GLN	2.1
1	A	166	SER	2.1
1	A	75	SER	2.0

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.

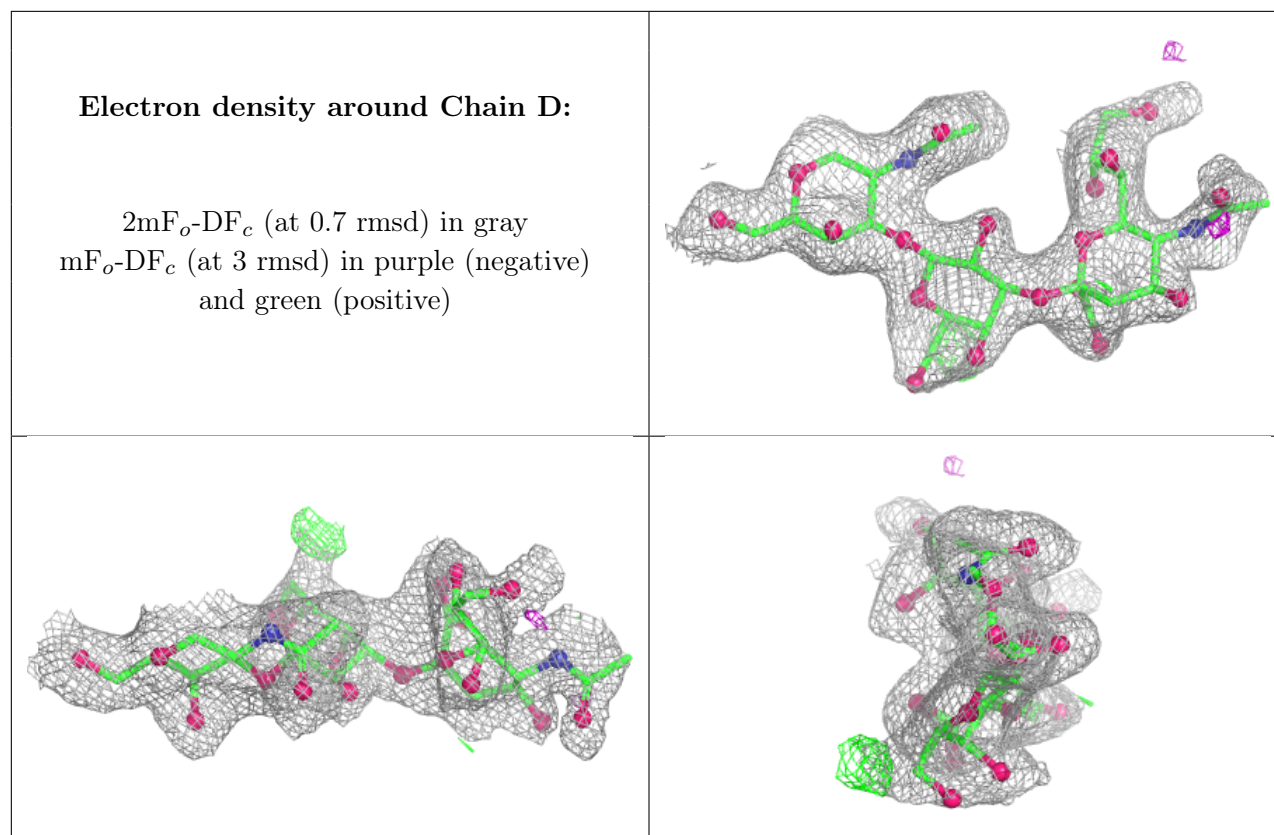
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MLY	B	174	11/12	0.82	0.17	36,43,63,63	0
2	MLY	B	79	11/12	0.85	0.15	29,32,52,57	0
2	MLY	B	112	11/12	0.88	0.14	33,40,60,62	0
1	MLY	A	74	11/12	0.88	0.14	45,49,64,64	0
1	MLY	A	214	11/12	0.89	0.13	40,44,59,65	0
2	MLY	B	188	11/12	0.89	0.12	33,40,57,63	0
1	MLY	A	19	11/12	0.90	0.12	34,38,50,52	0
2	MLY	B	204	11/12	0.90	0.11	34,40,49,53	0
1	MLY	A	38	11/12	0.91	0.13	27,38,55,55	0
1	MLY	A	120	11/12	0.91	0.13	29,33,50,50	0
1	MLY	A	67	11/12	0.92	0.12	32,38,48,49	0
2	MLY	B	212	11/12	0.92	0.12	31,36,58,60	0
1	MLY	A	213	11/12	0.93	0.10	37,42,45,46	0
1	MLY	A	148	11/12	0.93	0.11	29,31,37,41	0
2	MLY	B	50	11/12	0.94	0.10	26,34,46,48	0
2	MLY	B	55	11/12	0.94	0.10	26,30,39,43	0
2	MLY	B	44	11/12	0.95	0.09	27,32,45,48	0
2	MLY	B	147	11/12	0.95	0.08	30,34,41,45	0
2	MLY	B	152	11/12	0.95	0.09	29,33,52,52	0
2	MLY	B	154	11/12	0.95	0.09	29,36,41,42	0

6.3 Carbohydrates

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	A2G	D	1	14/15	-	-	33,35,41,42	0
3	GAL	D	2	11/12	-	-	46,52,59,61	0
3	SIA	D	3	20/21	-	-	54,62,70,71	0

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



6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
10	PEG	B	304	7/7	0.75	0.18	46,48,54,55	0
11	GOL	A	510	6/6	0.78	0.14	53,56,61,65	0
10	PEG	A	508	7/7	0.82	0.15	45,47,54,56	0
10	PEG	B	305	7/7	0.83	0.15	47,49,53,54	0
11	GOL	A	509	6/6	0.84	0.20	38,42,47,55	0
10	PEG	A	507	7/7	0.87	0.12	37,42,45,50	0
10	PEG	B	307	7/7	0.87	0.13	44,45,48,54	0
10	PEG	B	303	7/7	0.88	0.13	39,45,49,54	0
13	LPD	B	302	8/8	0.91	0.08	35,38,43,49	0
9	TRS	A	506	8/8	0.93	0.08	34,35,37,40	0
5	ASP	A	502	8/9	0.94	0.08	34,36,37,38	0
12	PRO	B	301	7/8	0.94	0.08	30,31,34,35	0
10	PEG	B	306	7/7	0.94	0.09	42,47,49,50	0
4	N7P	A	501	10/11	0.95	0.09	40,42,51,53	0

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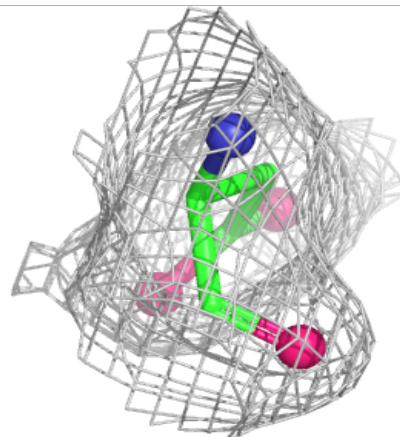
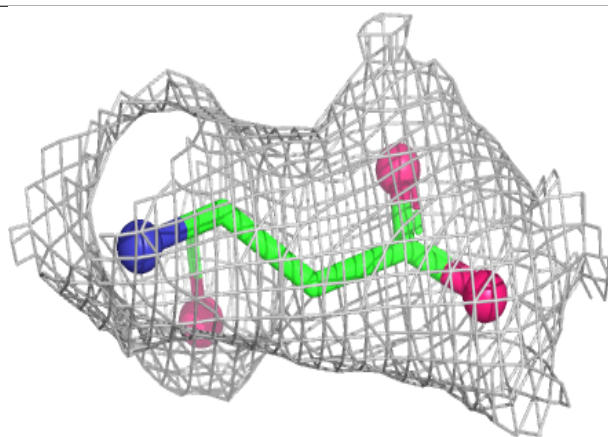
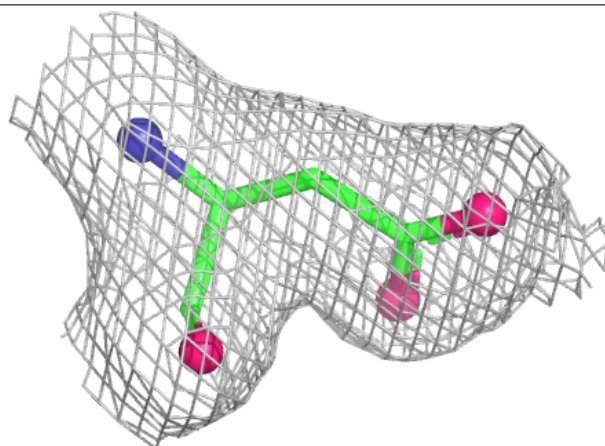
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	THR	A	503	7/8	0.96	0.08	32,33,35,37	0
7	ARG	A	504	11/12	0.97	0.05	26,28,33,34	0
8	ALA	A	505	5/6	0.97	0.06	35,35,37,38	0

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.

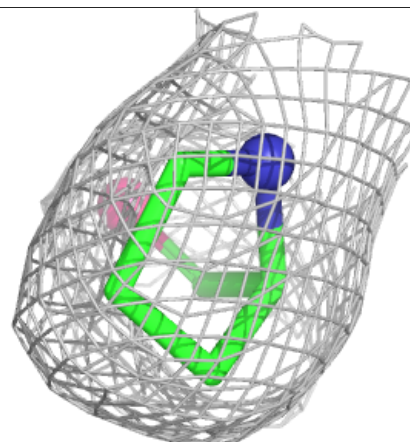
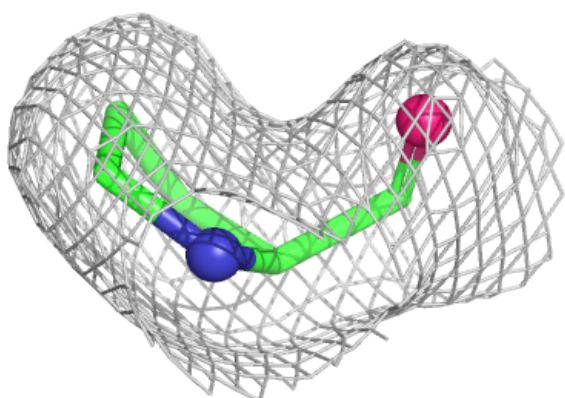
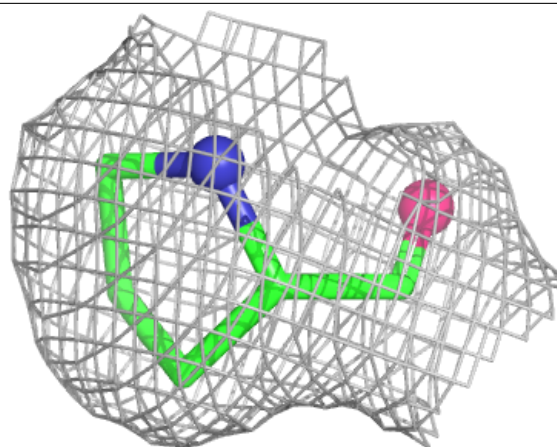
Electron density around ASP A 502:

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



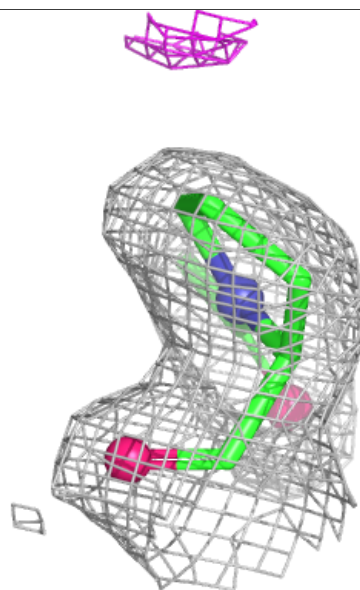
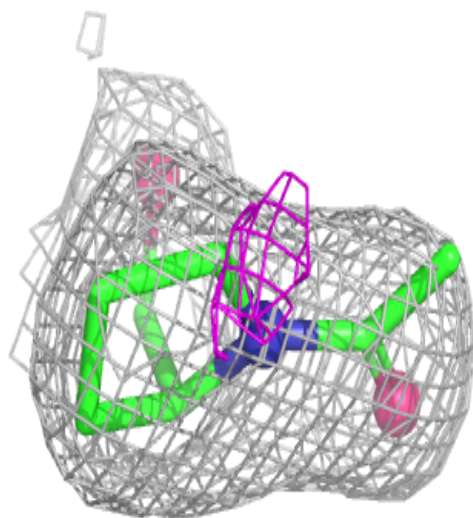
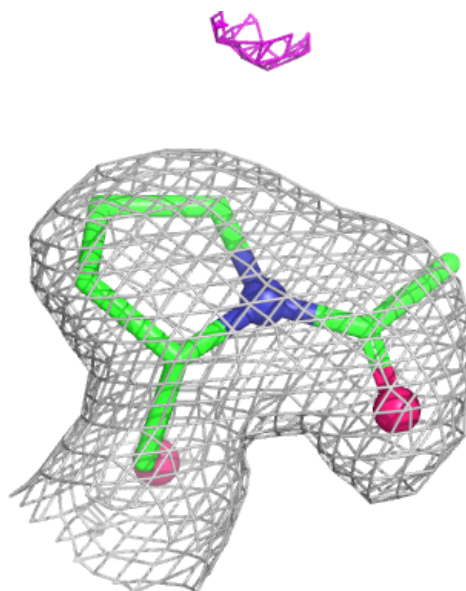
Electron density around PRO B 301:

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



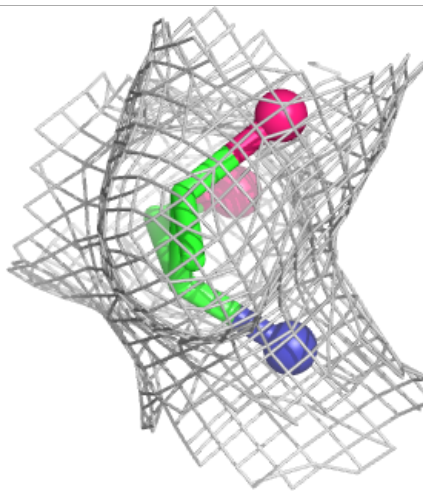
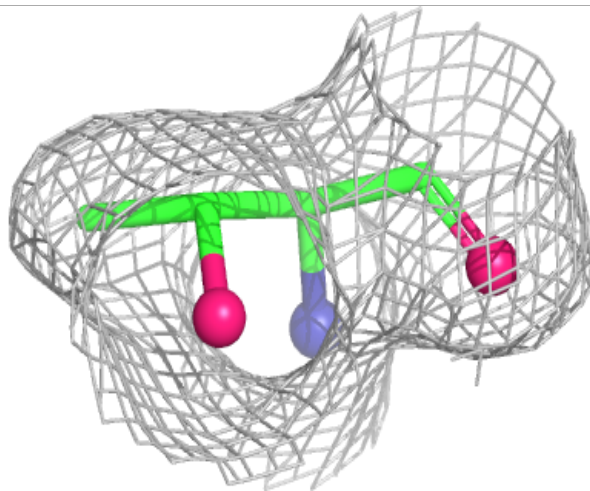
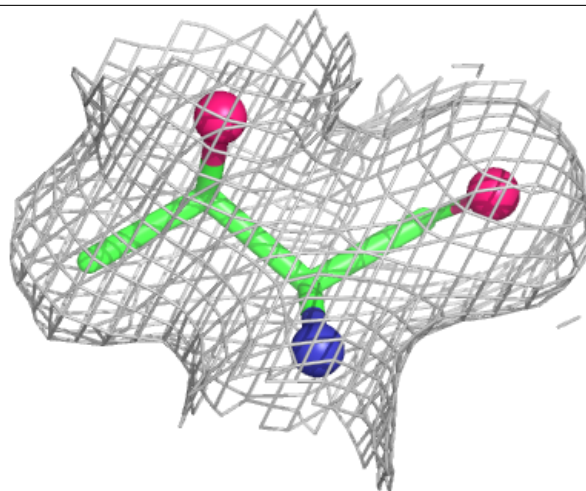
Electron density around N7P A 501:

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



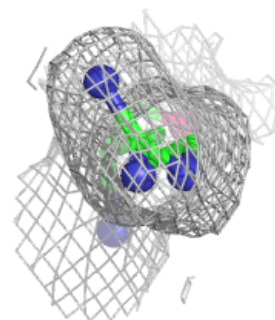
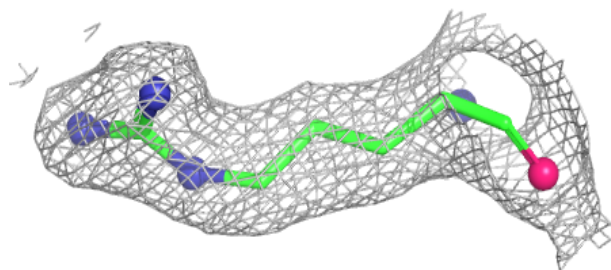
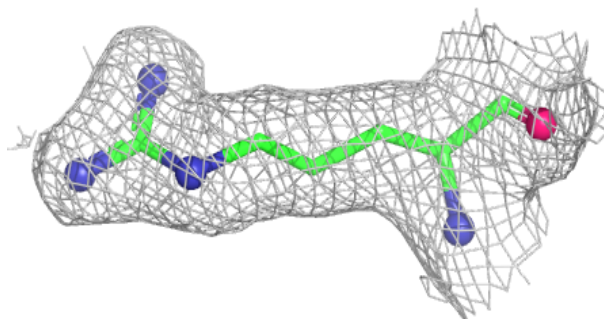
Electron density around THR A 503:

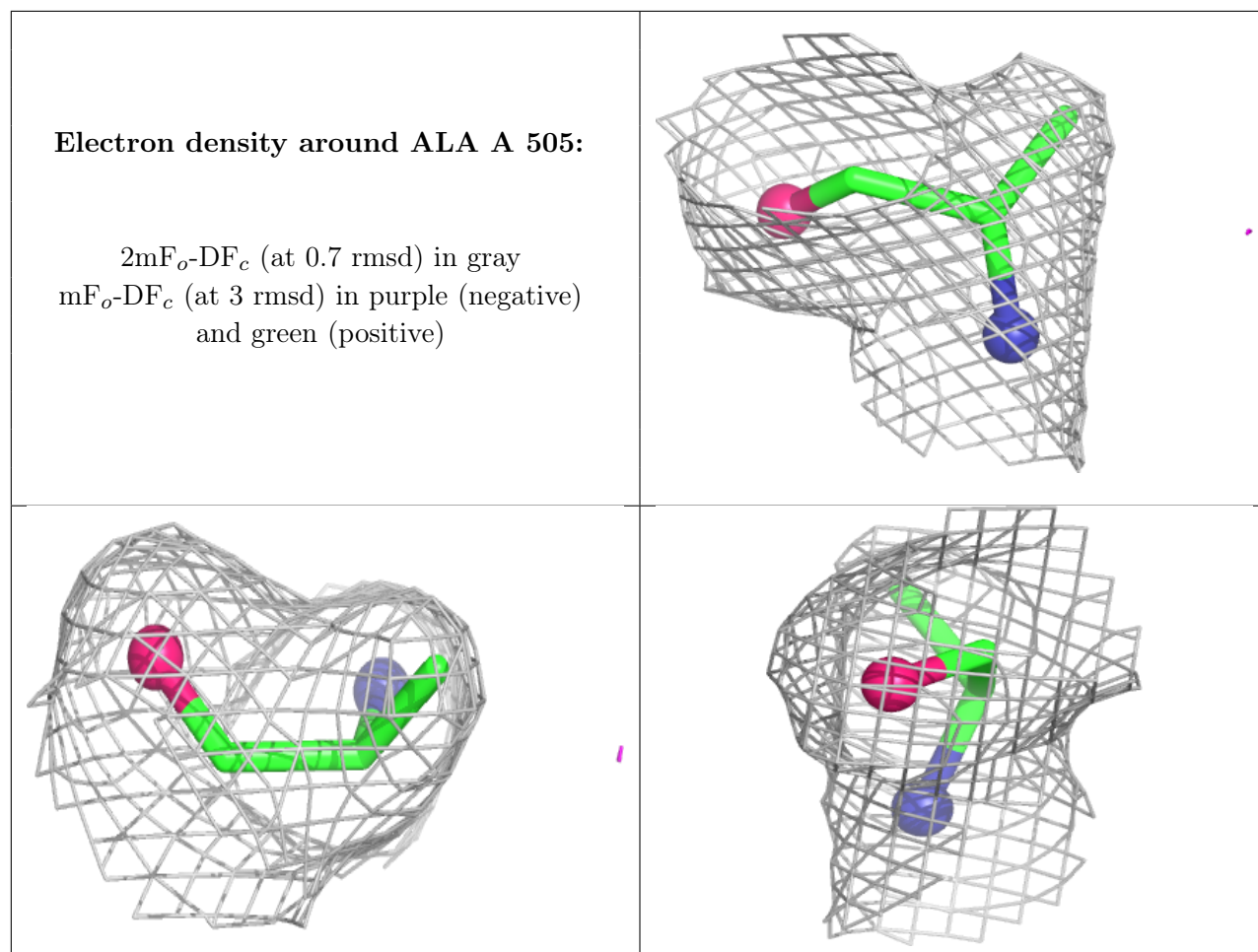
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.