



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:57 AM UTC

PDB ID : 4RER / pdb_00004rer
Title : Crystal structure of the phosphorylated human alpha1 beta2 gamma1 holo-AMPK complex bound to AMP and cyclodextrin
Authors : Zhou, X.E.; Ke, J.; Li, X.; Wang, L.; Gu, X.; de Waal, P.W.; Tan, M.H.E.; Wang, D.; Wu, D.; Xu, H.E.; Melcher, K.
Deposited on : 2014-09-23
Resolution : 4.05 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

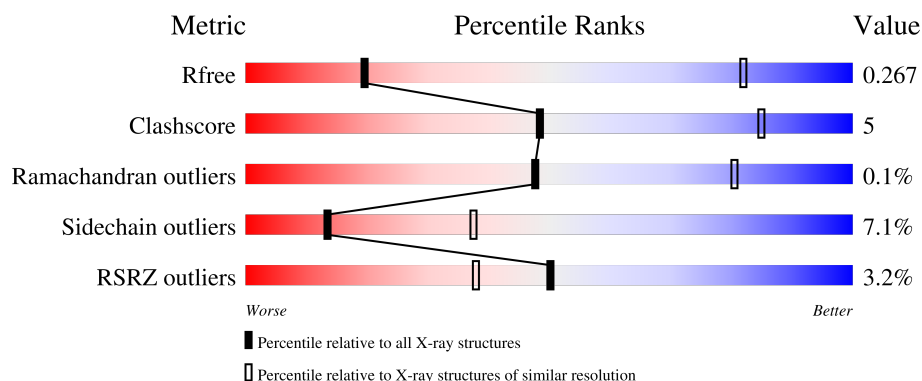
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.05 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	1117 (4.28-3.80)
Clashscore	190562	1164 (4.28-3.80)
Ramachandran outliers	187476	1095 (4.28-3.80)
Sidechain outliers	187428	1086 (4.28-3.80)
RSRZ outliers	180081	1117 (4.28-3.80)

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	540	2% 68% 15% . 15%
2	B	197	5% 72% 19% . 8%
3	G	304	3% 82% 15% ..
4	C	7	100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7798 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 5'-AMP-activated protein kinase catalytic subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	P	S	0	0	0
			3725	2376	649	677	1	22			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	SER	ARG	conflict	UNP Q13131
A	260	SER	THR	conflict	UNP Q13131
A	471	GLY	GLU	engineered mutation	UNP Q13131
A	474	ALA	GLU	engineered mutation	UNP Q13131
A	476	ALA	LYS	engineered mutation	UNP Q13131

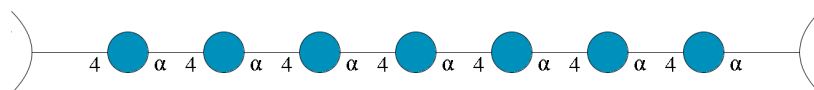
- Molecule 2 is a protein called 5'-AMP-activated protein kinase subunit beta-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	P	S	0	0	0
			1458	945	240	268	1	4			

- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

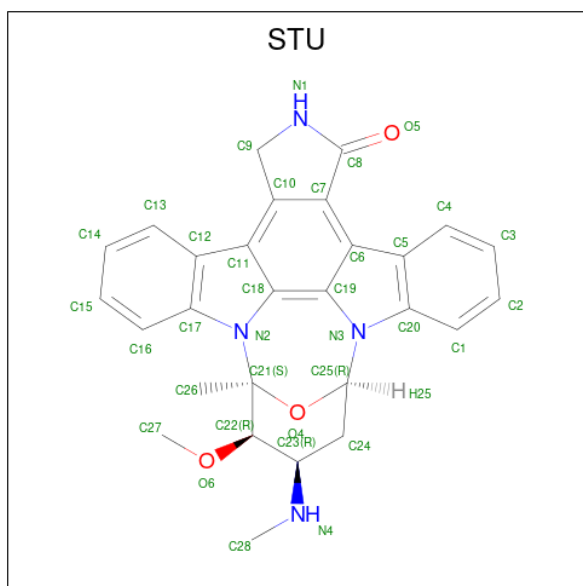
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	300	Total	C	N	O	S	0	0	0
			2419	1571	403	438	7			

- Molecule 4 is an oligosaccharide called Cycloheptakis-(1-4)-(alpha-D-glucopyranose).



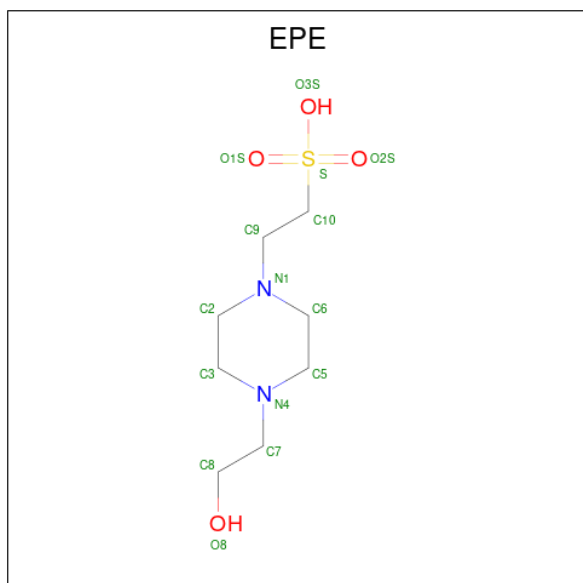
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	C	7	Total	C	O	0	0	0
			77	42	35			

- Molecule 5 is STAUROSPORINE (CCD ID: STU) (formula: $C_{28}H_{26}N_4O_3$).



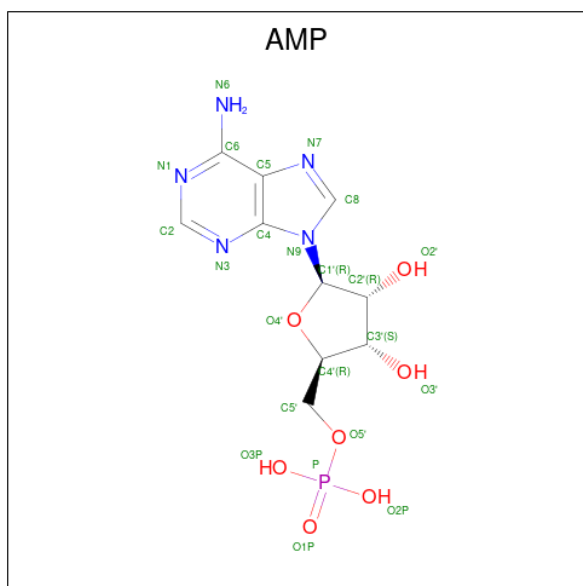
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).

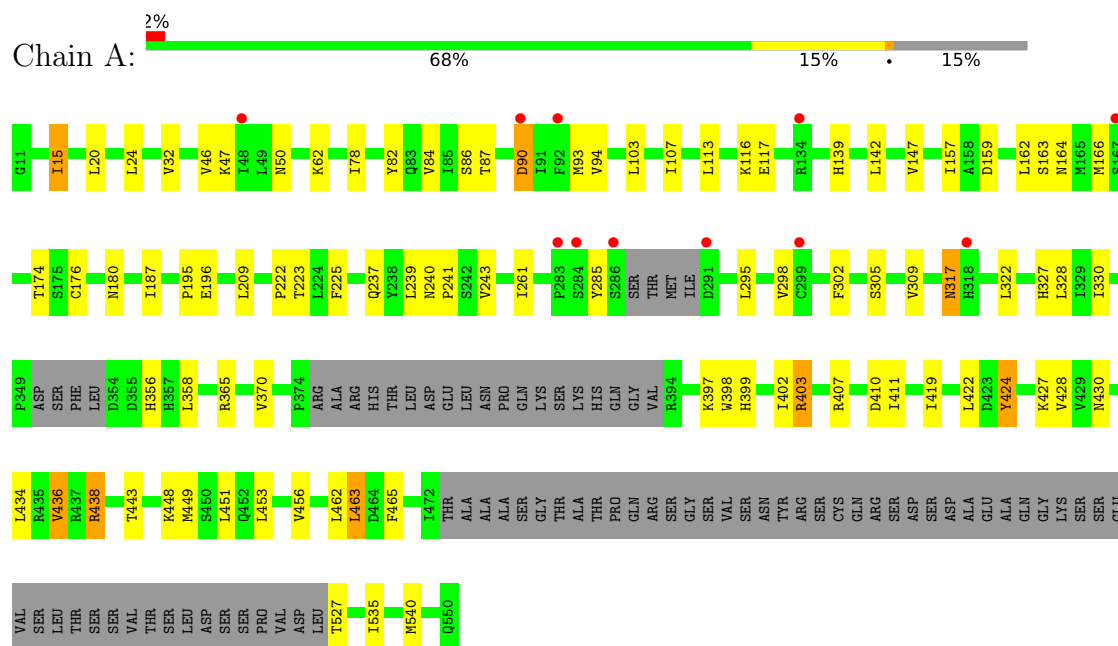


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
7	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
7	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

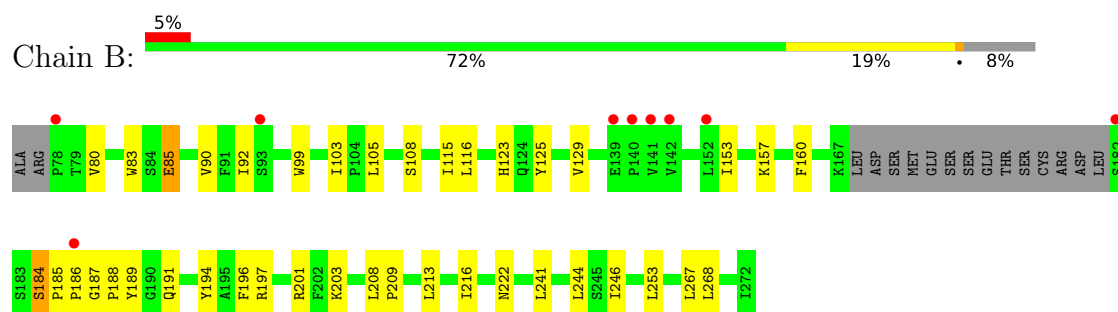
3 Residue-property plots [i](#)

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.

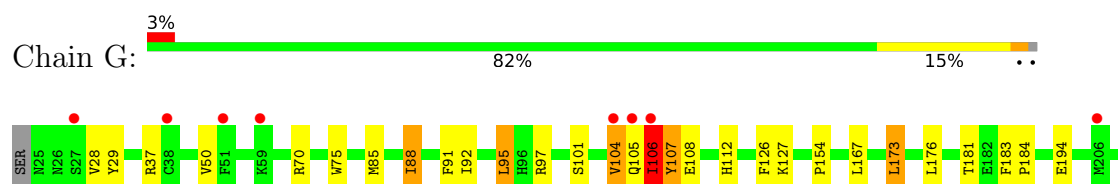
- Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-1



- Molecule 2: 5'-AMP-activated protein kinase subunit beta-2



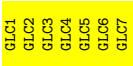
- Molecule 3: 5'-AMP-activated protein kinase subunit gamma-1





- Molecule 4: Cycloheptakis-(1-4)-(alpha-D-glucopyranose)

Chain C: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	132.57Å 132.57Å 195.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.66 – 4.05 39.66 – 4.05	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.66-4.05) 99.0 (39.66-4.05)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.224 , 0.260 0.239 , 0.267	Depositor DCC
R_{free} test set	1213 reflections (7.24%)	wwPDB-VP
Wilson B-factor (Å ²)	122.7	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 137.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	7798	wwPDB-VP
Average B, all atoms (Å ²)	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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: STU, AMP, EPE, TPO, GLC, SEP

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	0.39	0/3800	0.77	4/5132 (0.1%)
2	B	0.43	2/1491 (0.1%)	0.87	4/2027 (0.2%)
3	G	0.39	0/2470	0.75	2/3353 (0.1%)
All	All	0.40	2/7761 (0.0%)	0.78	10/10512 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	187	GLY	C-N	5.72	1.41	1.33
2	B	188	PRO	N-CD	5.05	1.54	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	104	VAL	N-CA-C	8.12	118.21	110.42
2	B	184	SER	CA-C-N	-7.17	112.99	120.38
2	B	184	SER	C-N-CA	-7.17	112.99	120.38
3	G	107	TYR	N-CA-C	7.13	118.70	111.07
2	B	187	GLY	CA-C-N	-6.73	113.05	119.85
2	B	187	GLY	C-N-CA	-6.73	113.05	119.85
1	A	527	THR	CA-C-N	-6.55	113.78	120.85
1	A	527	THR	C-N-CA	-6.55	113.78	120.85
1	A	295	LEU	CA-C-N	-5.09	115.23	122.41
1	A	295	LEU	C-N-CA	-5.09	115.23	122.41

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	3725	0	3716	44	0
2	B	1458	0	1446	16	0
3	G	2419	0	2483	27	0
4	C	77	0	61	0	0
5	A	35	0	26	3	0
6	A	15	0	17	1	0
7	G	69	0	36	1	0
All	All	7798	0	7785	85	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 5.

All (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:TYR:CD2	1:A:438:ARG:HB3	2.12	0.85
1:A:32:VAL:HG12	1:A:47:LYS:HA	1.76	0.68
3:G:101:SER:HB3	3:G:104:VAL:HG22	1.75	0.66
3:G:301:VAL:HG12	3:G:312:ILE:HG12	1.80	0.64
3:G:173:LEU:HD12	3:G:315:LEU:HD22	1.80	0.64
2:B:83:TRP:NE1	2:B:85:GLU:O	2.32	0.63
1:A:403:ARG:HG3	1:A:462:LEU:HD23	1.81	0.62
1:A:428:VAL:HG12	1:A:434:LEU:HG	1.84	0.59
1:A:438:ARG:HG2	1:A:540:MET:HE2	1.84	0.59
1:A:139:HIS:NE2	1:A:159:ASP:O	2.36	0.58
5:A:601:STU:H261	5:A:601:STU:H16	1.85	0.58
1:A:187:ILE:HD13	1:A:225:PHE:HB3	1.86	0.57
1:A:456:VAL:HG12	2:B:208:LEU:HD22	1.86	0.56
1:A:317:ASN:OD1	1:A:317:ASN:N	2.32	0.56
2:B:90:VAL:HG12	2:B:129:VAL:HG12	1.88	0.56
1:A:239:LEU:HD13	1:A:243:VAL:HB	1.88	0.55
3:G:302:VAL:HG23	3:G:310:LYS:HB2	1.90	0.54
3:G:244:PHE:HB3	7:G:402:AMP:H5'1	1.91	0.53
3:G:194:GLU:HB2	3:G:281:LEU:HB3	1.89	0.53
1:A:407:ARG:HB2	1:A:410:ASP:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:LEU:HD11	2:B:253:LEU:HD12	1.89	0.52
3:G:226:SER:HA	3:G:243:LYS:HD3	1.90	0.52
1:A:113:LEU:HD12	1:A:117:GLU:HG2	1.93	0.51
1:A:398:TRP:CD1	2:B:244:LEU:HB2	2.45	0.51
2:B:90:VAL:HG23	2:B:105:LEU:HB2	1.93	0.50
3:G:279:CYS:SG	3:G:302:VAL:HG12	2.52	0.49
2:B:103:ILE:HG13	2:B:116:LEU:HD11	1.92	0.49
1:A:451:LEU:HB3	1:A:463:LEU:HD21	1.93	0.49
3:G:91:PHE:O	3:G:95:LEU:HB2	2.13	0.48
3:G:105:GLN:O	3:G:106:ILE:HG12	2.13	0.48
1:A:422:LEU:HB3	1:A:424:TYR:CD1	2.49	0.48
1:A:424:TYR:CD1	1:A:424:TYR:N	2.81	0.48
2:B:123:HIS:CE1	2:B:125:TYR:HB3	2.49	0.48
3:G:92:ILE:HG23	3:G:217:LEU:HD22	1.95	0.48
2:B:268:LEU:HD13	3:G:50:VAL:HG23	1.95	0.48
1:A:15:ILE:HG13	1:A:20:LEU:HD21	1.95	0.47
1:A:222:PRO:O	1:A:225:PHE:N	2.48	0.47
1:A:402:ILE:HG22	1:A:465:PHE:HE1	1.80	0.47
1:A:46:VAL:HG12	1:A:94:VAL:HG12	1.97	0.47
1:A:305:SER:O	1:A:309:VAL:HG22	2.15	0.46
1:A:424:TYR:CD2	1:A:438:ARG:CB	2.94	0.46
3:G:243:LYS:O	3:G:246:VAL:HG22	2.15	0.46
1:A:50:ASN:HA	1:A:90:ASP:HB3	1.97	0.46
1:A:365:ARG:NH1	2:B:222:ASN:O	2.48	0.46
1:A:327:HIS:O	1:A:330:ILE:HG22	2.15	0.46
1:A:196:GLU:OE1	1:A:196:GLU:N	2.43	0.46
1:A:424:TYR:N	1:A:424:TYR:HD1	2.13	0.45
1:A:24:LEU:HB2	1:A:32:VAL:HG23	1.98	0.45
3:G:220:PHE:CE1	3:G:243:LYS:HG3	2.51	0.45
1:A:162:LEU:HD23	1:A:176:CYS:SG	2.56	0.45
3:G:28:VAL:HG23	3:G:29:TYR:H	1.81	0.45
1:A:163:SER:OG	1:A:164:ASN:N	2.49	0.45
1:A:107:ILE:HD13	1:A:113:LEU:HD23	1.98	0.45
1:A:107:ILE:HD11	1:A:209:LEU:HD23	1.98	0.45
1:A:449:MET:HE2	1:A:451:LEU:HD11	1.99	0.44
2:B:184:SER:HB2	2:B:185:PRO:HD2	1.99	0.44
1:A:535:ILE:HG21	3:G:75:TRP:CE2	2.53	0.44
3:G:183:PHE:N	3:G:184:PRO:HD2	2.33	0.43
1:A:240:ASN:HB2	1:A:241:PRO:HD2	2.00	0.43
5:A:601:STU:HN4	5:A:601:STU:C18	2.31	0.43
1:A:84:VAL:HG12	1:A:93:MET:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:LEU:HD12	2:B:209:PRO:HD2	1.99	0.43
3:G:298:HIS:O	3:G:315:LEU:HG	2.17	0.43
1:A:411:ILE:HD11	1:A:453:LEU:HD21	2.01	0.43
1:A:436:VAL:HG22	1:A:449:MET:HG3	2.00	0.43
2:B:83:TRP:CZ2	2:B:129:VAL:HG11	2.53	0.43
1:A:82:TYR:HB2	1:A:94:VAL:HG23	1.99	0.43
1:A:78:ILE:HD13	1:A:157:ILE:HB	2.01	0.43
3:G:92:ILE:HG12	3:G:246:VAL:HG21	2.00	0.43
3:G:70:ARG:HE	3:G:88:ILE:HD11	1.83	0.42
1:A:166:MET:HE1	1:A:195:PRO:HG3	2.01	0.42
3:G:212:PRO:O	3:G:215:VAL:HG22	2.19	0.42
3:G:85:MET:HE3	3:G:154:PRO:HG3	2.02	0.42
6:A:602:EPE:H81	6:A:602:EPE:H52	1.85	0.41
3:G:271:HIS:HB3	3:G:272:TYR:CE1	2.55	0.41
5:A:601:STU:HN4	5:A:601:STU:C19	2.34	0.41
1:A:419:ILE:HD11	1:A:436:VAL:HG11	2.03	0.41
2:B:267:LEU:O	3:G:50:VAL:HG22	2.21	0.41
3:G:244:PHE:O	3:G:247:ILE:HG22	2.21	0.41
2:B:80:VAL:HG12	2:B:115:ILE:HG12	2.03	0.41
2:B:185:PRO:HA	2:B:186:PRO:HD3	1.81	0.40
1:A:103:LEU:HB2	1:A:147:VAL:HG23	2.03	0.40
3:G:92:ILE:CG1	3:G:246:VAL:HG21	2.52	0.40
1:A:298:VAL:HG11	1:A:305:SER:HB3	2.03	0.40
3:G:292:LEU:HD13	3:G:300:LEU:HG	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	448/540 (83%)	426 (95%)	22 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	176/197 (89%)	165 (94%)	11 (6%)	0	100	100
3	G	298/304 (98%)	285 (96%)	12 (4%)	1 (0%)	36	69
All	All	922/1041 (89%)	876 (95%)	45 (5%)	1 (0%)	48	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	106	ILE

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	414/484 (86%)	384 (93%)	30 (7%)	13	37
2	B	166/181 (92%)	150 (90%)	16 (10%)	8	27
3	G	275/278 (99%)	260 (94%)	15 (6%)	19	43
All	All	855/943 (91%)	794 (93%)	61 (7%)	13	37

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	62	LYS
1	A	86	SER
1	A	87	THR
1	A	90	ASP
1	A	116	LYS
1	A	142	LEU
1	A	180	ASN
1	A	223	THR
1	A	237	GLN
1	A	261	ILE
1	A	285	TYR
1	A	302	PHE

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Mol	Chain	Res	Type
1	A	317	ASN
1	A	322	LEU
1	A	328	LEU
1	A	356	HIS
1	A	358	LEU
1	A	370	VAL
1	A	397	LYS
1	A	399	HIS
1	A	403	ARG
1	A	424	TYR
1	A	427	LYS
1	A	430	ASN
1	A	436	VAL
1	A	438	ARG
1	A	443	THR
1	A	448	LYS
1	A	463	LEU
2	B	85	GLU
2	B	92	ILE
2	B	99	TRP
2	B	153	ILE
2	B	157	LYS
2	B	160	PHE
2	B	189	TYR
2	B	191	GLN
2	B	194	TYR
2	B	196	PHE
2	B	197	ARG
2	B	201	ARG
2	B	203	LYS
2	B	213	LEU
2	B	216	ILE
2	B	246	ILE
3	G	37	ARG
3	G	88	ILE
3	G	95	LEU
3	G	97	ARG
3	G	106	ILE
3	G	107	TYR
3	G	108	GLU
3	G	112	HIS
3	G	126	PHE

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Mol	Chain	Res	Type
3	G	127	LYS
3	G	167	LEU
3	G	173	LEU
3	G	176	LEU
3	G	181	THR
3	G	299	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	318	HIS
1	A	332	ASN
2	B	97	ASN
2	B	154	HIS
3	G	26	ASN
3	G	248	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	SEP	B	108	2	8,9,10	1.60	1 (12%)	7,12,14	0.88	0
1	TPO	A	174	1	8,10,11	1.05	0	10,14,16	1.88	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	SEP	B	108	2	-	0/6/8/10	-
1	TPO	A	174	1	-	0/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	108	SEP	P-O1P	3.48	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	TPO	P-OG1-CB	-5.03	109.65	123.33
1	A	174	TPO	CG2-CB-CA	-2.43	108.53	113.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

7 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
4	GLC	C	1	4	11,11,12	2.18	4 (36%)	15,15,17	1.28	2 (13%)
4	GLC	C	2	4	11,11,12	1.30	1 (9%)	15,15,17	1.03	1 (6%)
4	GLC	C	3	4	11,11,12	1.80	4 (36%)	15,15,17	1.11	1 (6%)
4	GLC	C	4	4	11,11,12	1.18	1 (9%)	15,15,17	1.27	1 (6%)
4	GLC	C	5	4	11,11,12	2.04	6 (54%)	15,15,17	1.49	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GLC	C	6	4	11,11,12	1.77	4 (36%)	15,15,17	2.07	3 (20%)
4	GLC	C	7	4	11,11,12	1.45	2 (18%)	15,15,17	1.75	2 (13%)

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	GLC	C	1	4	-	2/2/19/22	0/1/1/1
4	GLC	C	2	4	-	0/2/19/22	0/1/1/1
4	GLC	C	3	4	-	0/2/19/22	0/1/1/1
4	GLC	C	4	4	-	2/2/19/22	0/1/1/1
4	GLC	C	5	4	-	2/2/19/22	0/1/1/1
4	GLC	C	6	4	-	2/2/19/22	0/1/1/1
4	GLC	C	7	4	-	2/2/19/22	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	GLC	O5-C5	4.07	1.51	1.43
4	C	5	GLC	O2-C2	-3.76	1.35	1.43
4	C	1	GLC	C4-C3	-3.68	1.42	1.52
4	C	6	GLC	O2-C2	-3.47	1.36	1.43
4	C	3	GLC	C4-C3	-3.35	1.43	1.52
4	C	2	GLC	O5-C1	-3.15	1.38	1.43
4	C	7	GLC	O5-C1	-3.01	1.38	1.43
4	C	1	GLC	O4-C4	2.86	1.50	1.43
4	C	5	GLC	O5-C1	-2.82	1.39	1.43
4	C	7	GLC	O2-C2	-2.81	1.37	1.43
4	C	5	GLC	O4-C4	2.60	1.49	1.43
4	C	4	GLC	O5-C1	-2.59	1.39	1.43
4	C	3	GLC	O5-C1	-2.55	1.39	1.43
4	C	5	GLC	C4-C3	-2.48	1.45	1.52
4	C	3	GLC	O2-C2	-2.47	1.38	1.43
4	C	6	GLC	O5-C1	-2.26	1.39	1.43
4	C	6	GLC	O4-C4	2.24	1.48	1.43
4	C	1	GLC	O5-C1	-2.22	1.40	1.43
4	C	6	GLC	C4-C5	-2.21	1.48	1.53
4	C	3	GLC	C1-C2	2.18	1.57	1.52
4	C	5	GLC	C1-C2	2.11	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5	GLC	C4-C5	-2.02	1.48	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	6	GLC	C1-O5-C5	5.86	120.03	112.19
4	C	7	GLC	C1-O5-C5	5.03	118.92	112.19
4	C	5	GLC	C3-C4-C5	2.98	115.64	110.23
4	C	6	GLC	C3-C4-C5	2.92	115.52	110.23
4	C	4	GLC	C1-O5-C5	2.83	115.98	112.19
4	C	5	GLC	C2-C3-C4	2.80	115.79	110.86
4	C	5	GLC	O5-C5-C4	2.34	116.52	110.83
4	C	6	GLC	O5-C5-C4	2.31	116.45	110.83
4	C	1	GLC	C2-C3-C4	2.17	114.67	110.86
4	C	7	GLC	C1-C2-C3	2.09	112.68	109.64
4	C	3	GLC	C1-O5-C5	2.08	114.97	112.19
4	C	2	GLC	C1-O5-C5	2.06	114.94	112.19
4	C	5	GLC	C1-O5-C5	2.05	114.94	112.19
4	C	1	GLC	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

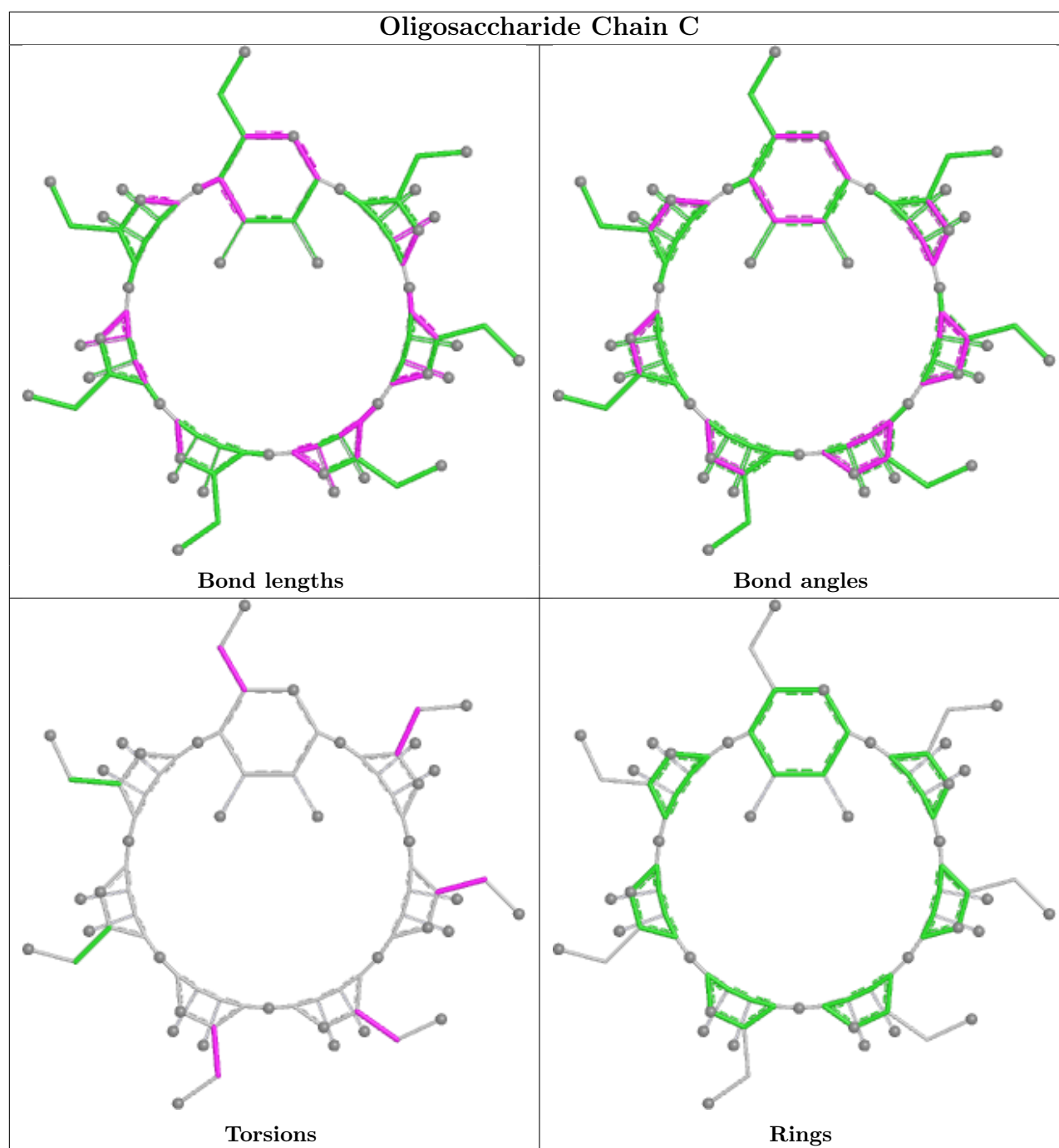
All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	4	GLC	O5-C5-C6-O6
4	C	6	GLC	O5-C5-C6-O6
4	C	7	GLC	O5-C5-C6-O6
4	C	4	GLC	C4-C5-C6-O6
4	C	5	GLC	C4-C5-C6-O6
4	C	5	GLC	O5-C5-C6-O6
4	C	1	GLC	C4-C5-C6-O6
4	C	7	GLC	C4-C5-C6-O6
4	C	6	GLC	C4-C5-C6-O6
4	C	1	GLC	O5-C5-C6-O6

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](#)

5 ligands are modelled in this entry.

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

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	STU	A	601	-	39,42,42	0.83	2 (5%)	50,68,68	2.24	11 (22%)
7	AMP	G	401	-	25,25,25	1.63	4 (16%)	37,38,38	1.85	10 (27%)
7	AMP	G	402	-	25,25,25	1.58	4 (16%)	37,38,38	1.91	9 (24%)
6	EPE	A	602	-	15,15,15	0.65	0	19,20,20	1.54	4 (21%)
7	AMP	G	403	-	25,25,25	1.60	4 (16%)	37,38,38	1.70	9 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	STU	A	601	-	-	2/4/42/42	-
7	AMP	G	401	-	-	0/10/26/26	0/3/3/3
7	AMP	G	402	-	-	0/10/26/26	0/3/3/3
6	EPE	A	602	-	-	2/9/19/19	0/1/1/1
7	AMP	G	403	-	-	0/10/26/26	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	401	AMP	C6-N6	5.86	1.49	1.34
7	G	403	AMP	C6-N6	5.75	1.48	1.34
7	G	402	AMP	C6-N6	5.74	1.48	1.34
7	G	401	AMP	P-O1P	3.14	1.60	1.50
7	G	403	AMP	P-O1P	3.05	1.60	1.50
7	G	401	AMP	P-O3P	-3.02	1.43	1.54
7	G	402	AMP	P-O3P	-2.96	1.43	1.54
7	G	402	AMP	P-O1P	2.93	1.59	1.50
7	G	403	AMP	P-O3P	-2.91	1.44	1.54
5	A	601	STU	O4-C25	-2.90	1.38	1.43
5	A	601	STU	C19-N3	-2.39	1.35	1.39
7	G	402	AMP	C8-N7	2.02	1.35	1.31
7	G	401	AMP	C8-N7	2.01	1.35	1.31
7	G	403	AMP	C8-N7	2.01	1.35	1.31

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	STU	C9-C10-C7	-8.43	106.79	109.88
7	G	402	AMP	C5-C4-N3	-5.61	118.99	126.72
7	G	401	AMP	C5-C4-N3	-5.58	119.03	126.72
7	G	403	AMP	C5-C4-N3	-5.55	119.07	126.72
5	A	601	STU	C9-N1-C8	-5.50	108.85	113.86
5	A	601	STU	C28-N4-C23	-4.95	108.47	114.39
5	A	601	STU	C10-C9-N1	4.42	106.05	101.75
5	A	601	STU	C27-O6-C22	-4.31	107.17	114.46
5	A	601	STU	C7-C8-N1	4.05	110.24	106.38
5	A	601	STU	C9-C10-C11	3.99	131.76	128.73
7	G	402	AMP	N3-C2-N1	-3.98	122.55	128.58
7	G	402	AMP	N3-C4-N9	3.93	133.85	127.17
7	G	401	AMP	N3-C4-N9	3.84	133.70	127.17
7	G	401	AMP	N3-C2-N1	-3.81	122.82	128.58
7	G	402	AMP	N9-C8-N7	-3.70	108.69	113.94
7	G	403	AMP	N3-C4-N9	3.50	133.12	127.17
6	A	602	EPE	C7-N4-C5	3.45	120.44	111.24
7	G	402	AMP	C2-N3-C4	3.38	120.08	111.83
6	A	602	EPE	C5-N4-C3	3.30	115.95	108.84
6	A	602	EPE	C6-N1-C2	3.29	115.93	108.84
7	G	403	AMP	N3-C2-N1	-3.21	123.72	128.58
7	G	402	AMP	C5-N7-C8	3.20	108.48	103.45
7	G	401	AMP	C2-N3-C4	3.14	119.50	111.83
7	G	402	AMP	C4-C5-N7	-3.09	107.05	110.58
7	G	401	AMP	N9-C8-N7	-3.08	109.57	113.94
7	G	403	AMP	C4-C5-N7	-3.00	107.15	110.58
7	G	403	AMP	C2-N3-C4	2.87	118.83	111.83
7	G	401	AMP	C4-C5-N7	-2.86	107.31	110.58
7	G	401	AMP	C5-N7-C8	2.84	107.92	103.45
5	A	601	STU	C16-C17-C12	-2.80	118.32	121.59
7	G	402	AMP	C4-N9-C8	2.75	108.62	105.74
7	G	403	AMP	C5-N7-C8	2.67	107.64	103.45
7	G	403	AMP	N9-C8-N7	-2.59	110.26	113.94
5	A	601	STU	C19-N3-C20	2.30	110.94	107.90
7	G	403	AMP	O2P-P-O1P	2.24	119.57	110.83
7	G	402	AMP	O2P-P-O1P	2.22	119.47	110.83
5	A	601	STU	C6-C7-C10	-2.18	119.24	120.76
7	G	403	AMP	C6-C5-C4	2.17	120.15	117.18
7	G	401	AMP	O2P-P-O1P	2.17	119.30	110.83
5	A	601	STU	C13-C12-C17	2.11	121.67	119.24
6	A	602	EPE	C7-N4-C3	2.08	116.78	111.24
7	G	401	AMP	C4-N9-C8	2.08	107.92	105.74
7	G	401	AMP	C6-C5-C4	2.04	119.97	117.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	STU	C22-C23-N4-C28
6	A	602	EPE	C8-C7-N4-C5
5	A	601	STU	C24-C23-N4-C28
6	A	602	EPE	C10-C9-N1-C6

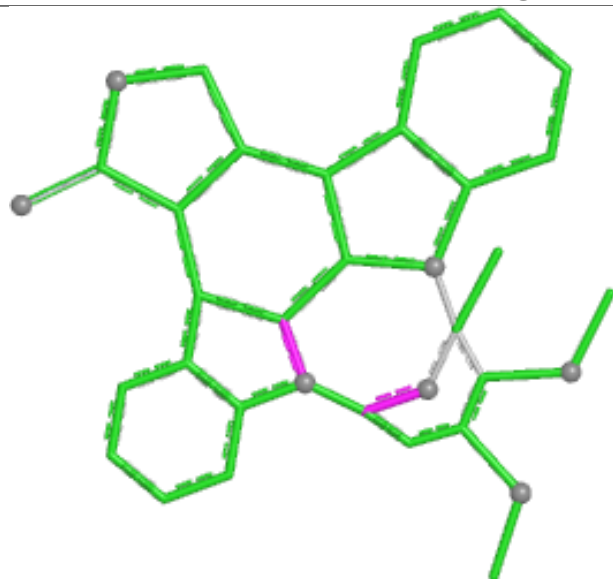
There are no ring outliers.

3 monomers are involved in 5 short contacts:

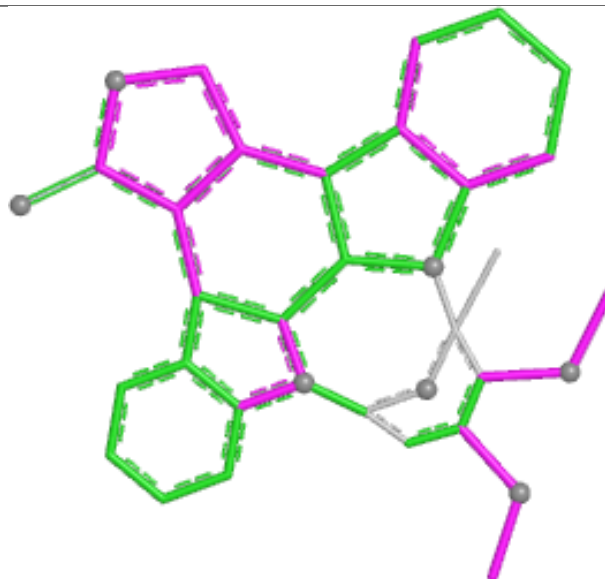
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	STU	3	0
7	G	402	AMP	1	0
6	A	602	EPE	1	0

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 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.

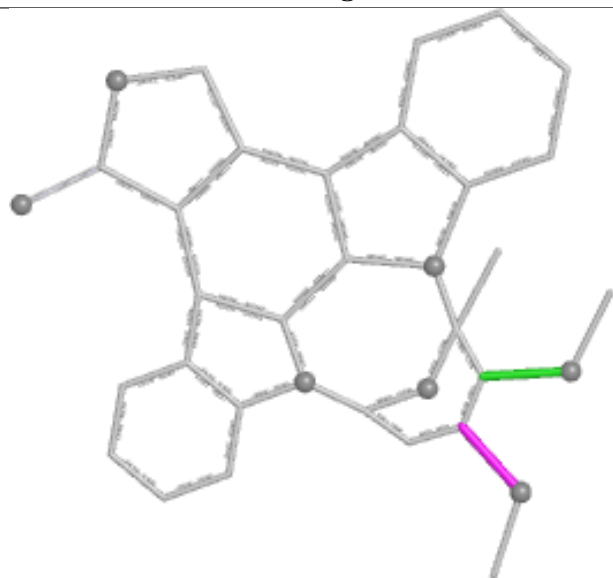
Ligand STU A 601



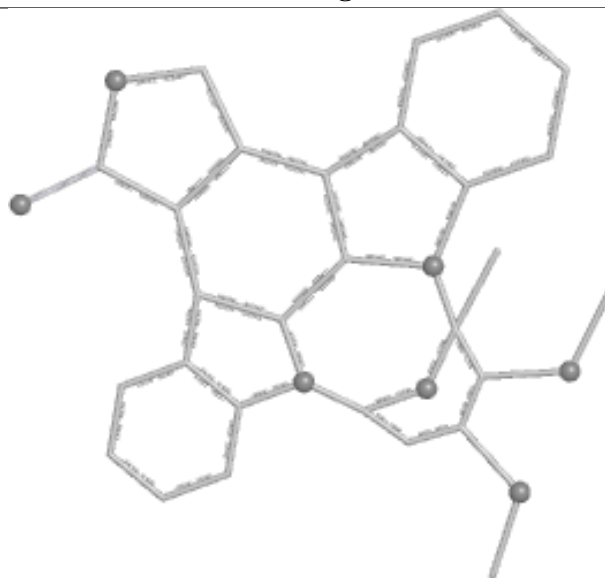
Bond lengths



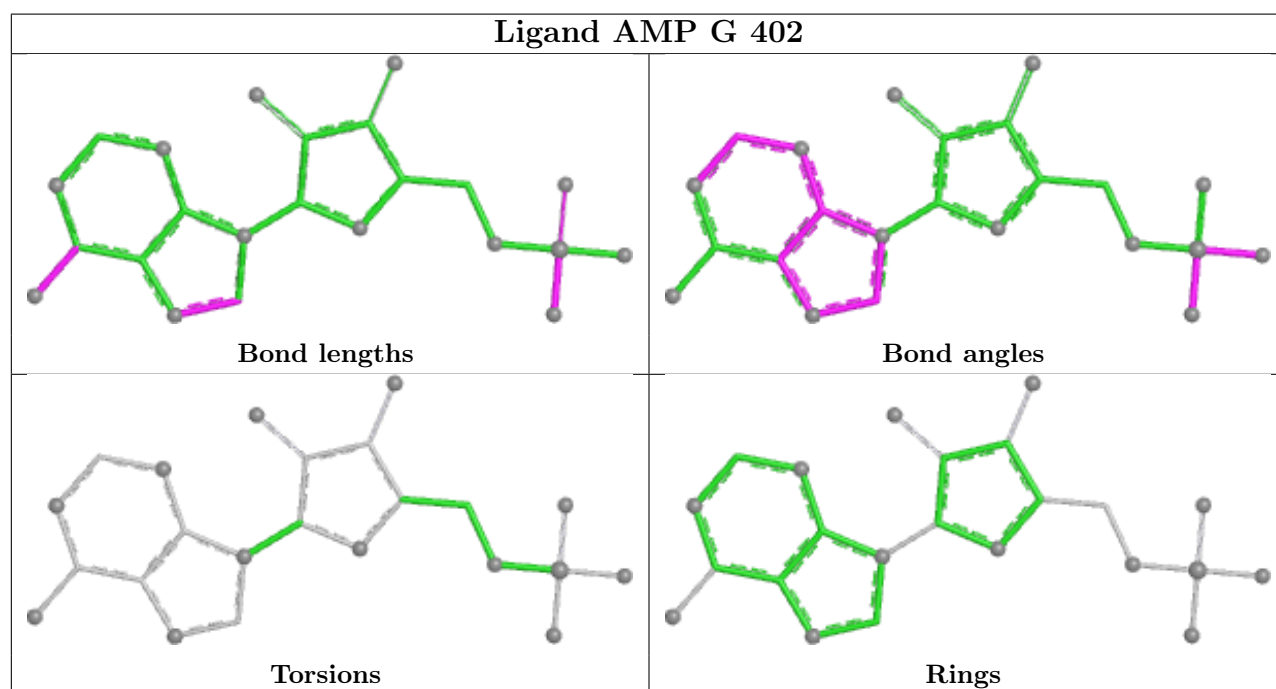
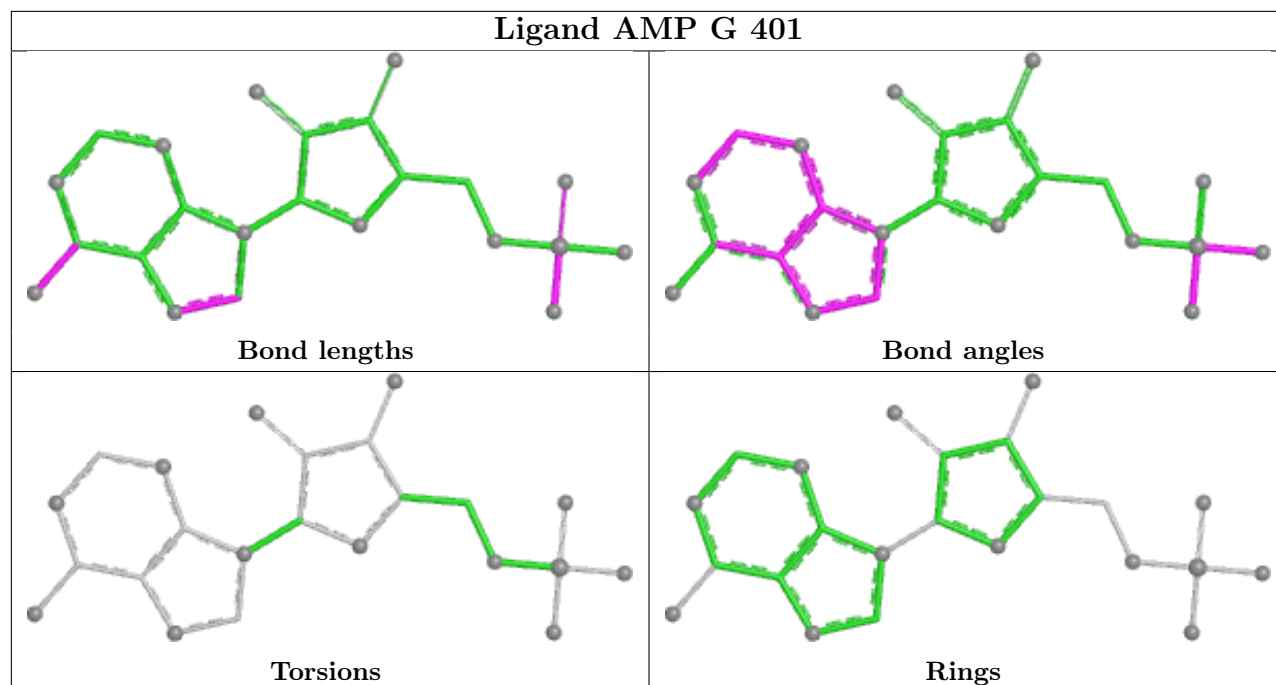
Bond angles

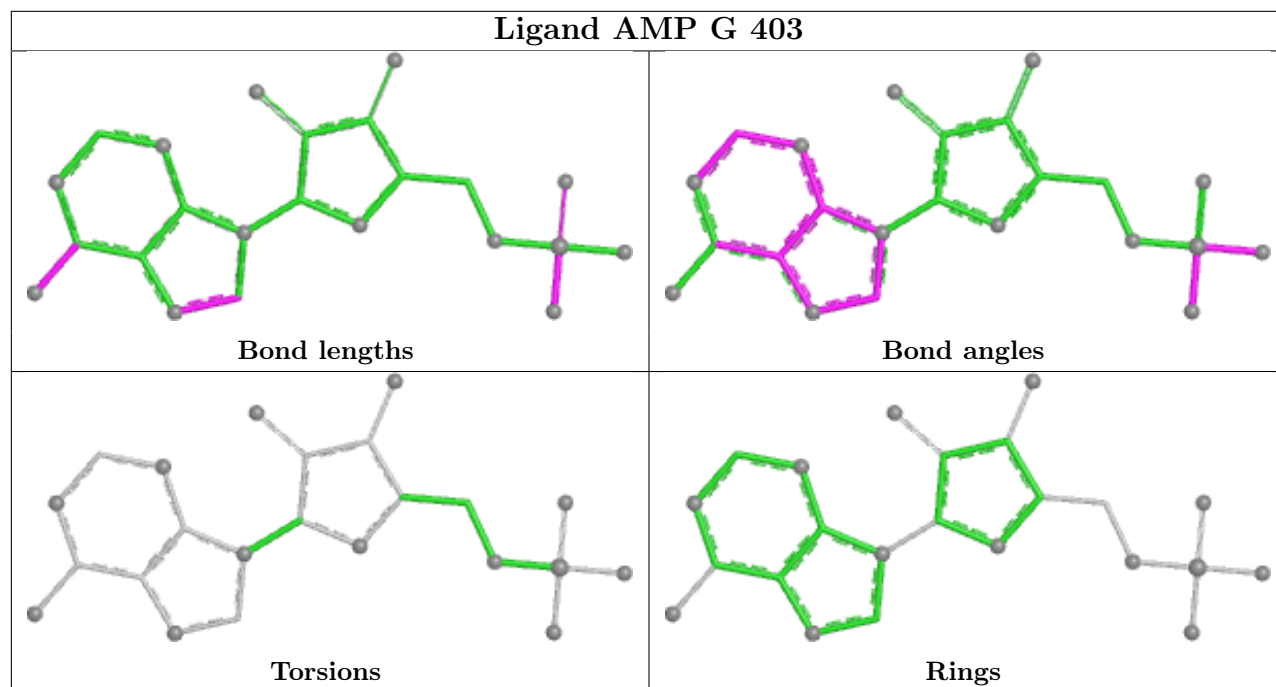


Torsions



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	458/540 (84%)	0.49	11 (2%) 59 45	108, 154, 287, 409	0
2	B	180/197 (91%)	0.62	9 (5%) 34 28	120, 220, 314, 361	0
3	G	300/304 (98%)	0.31	10 (3%) 49 37	98, 132, 212, 332	0
All	All	938/1041 (90%)	0.46	30 (3%) 50 38	98, 151, 281, 409	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291	ASP	5.8
1	A	286	SER	3.9
1	A	318	HIS	3.4
3	G	306	ASN	3.4
3	G	105	GLN	3.3
2	B	141	VAL	3.1
3	G	27	SER	3.0
3	G	274	GLU	2.9
1	A	284	SER	2.9
2	B	139	GLU	2.9
2	B	142	VAL	2.8
2	B	78	PRO	2.8
1	A	90	ASP	2.8
2	B	182	SER	2.7
2	B	93	SER	2.6
1	A	48	ILE	2.6
3	G	104	VAL	2.5
2	B	186	PRO	2.5
3	G	51	PHE	2.4
2	B	140	PRO	2.4
3	G	206	MET	2.4
3	G	38	CYS	2.4
1	A	167	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	299	CYS	2.2
3	G	106	ILE	2.2
1	A	283	PRO	2.2
1	A	92	PHE	2.2
1	A	134	ARG	2.1
2	B	152	LEU	2.1
3	G	59	LYS	2.1

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.

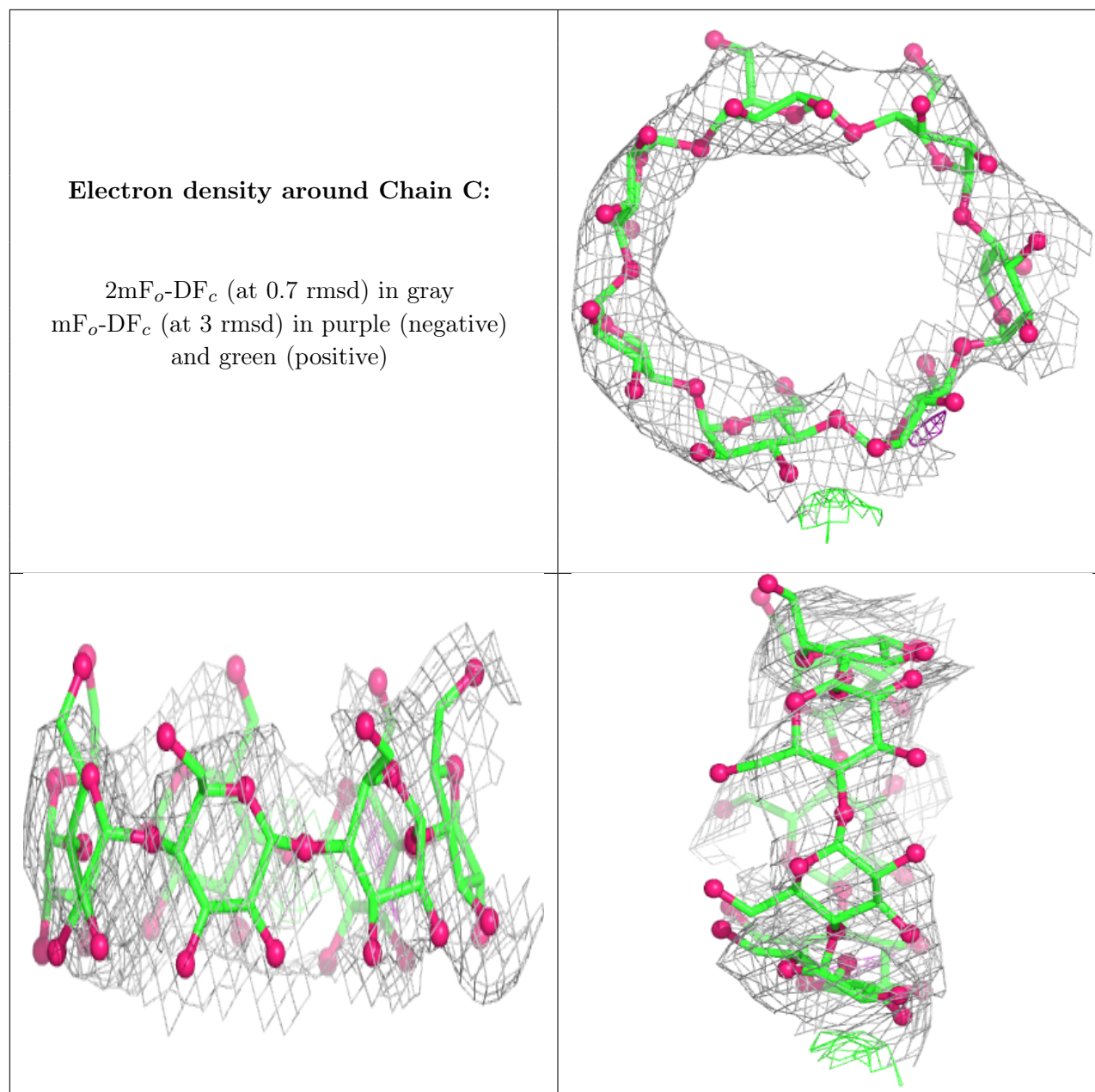
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SEP	B	108	10/11	0.50	0.15	222,225,311,311	0
1	TPO	A	174	11/12	0.94	0.11	123,136,138,138	0

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
4	GLC	C	1	11/12	-	-	243,247,251,251	0
4	GLC	C	2	11/12	-	-	235,238,240,241	0
4	GLC	C	3	11/12	-	-	233,236,241,242	0
4	GLC	C	4	11/12	-	-	238,243,247,247	0
4	GLC	C	5	11/12	-	-	249,253,255,256	0
4	GLC	C	6	11/12	-	-	257,258,263,265	0
4	GLC	C	7	11/12	-	-	252,256,260,260	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 [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
6	EPE	A	602	15/15	0.82	0.13	160,165,172,173	0
5	STU	A	601	35/35	0.92	0.12	121,124,127,127	0
7	AMP	G	401	23/23	0.93	0.12	117,127,154,156	0

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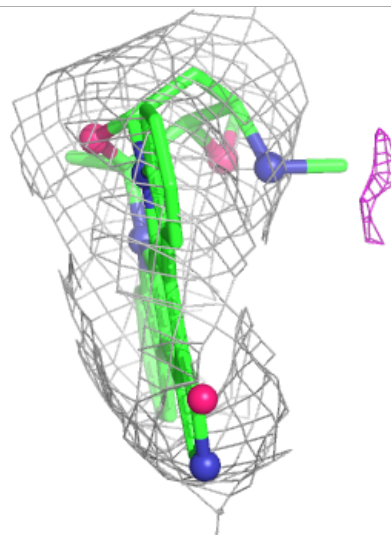
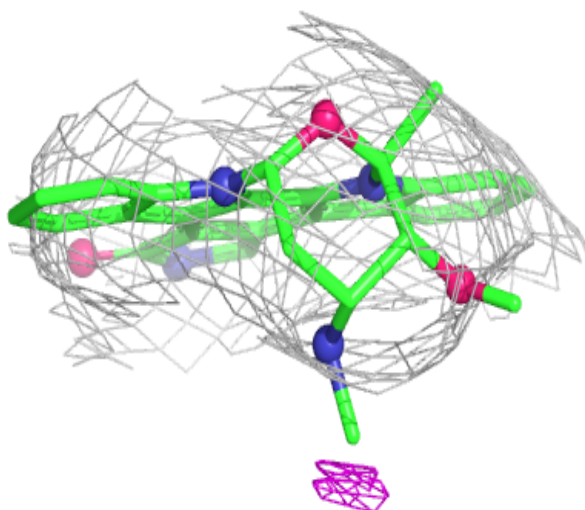
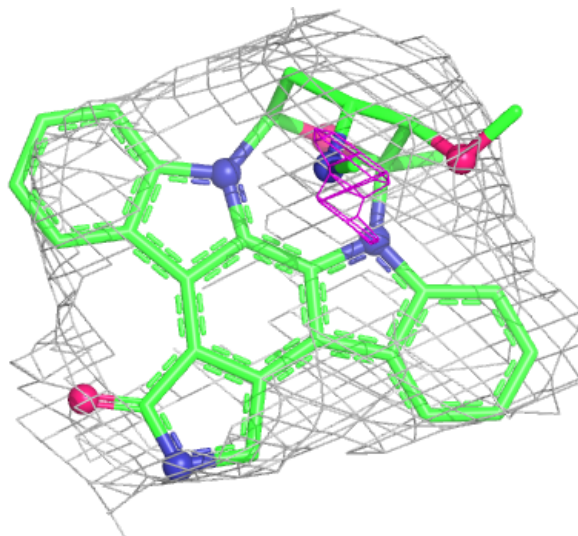
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	AMP	G	402	23/23	0.94	0.12	99,101,128,129	0
7	AMP	G	403	23/23	0.94	0.12	111,122,131,133	0

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.

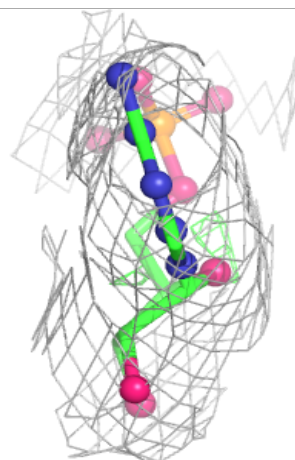
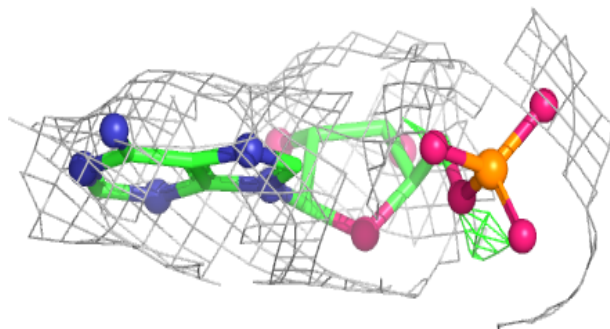
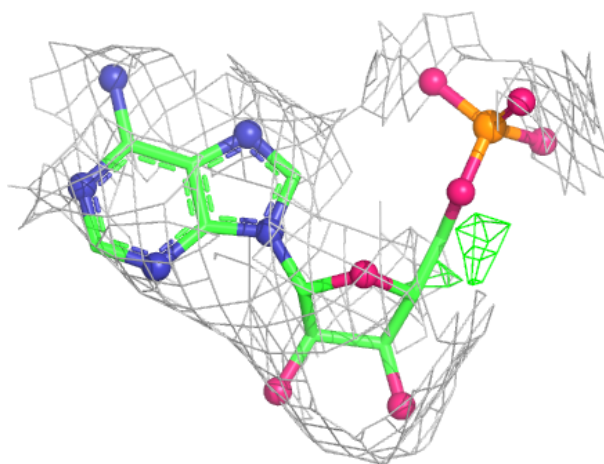
Electron density around STU A 601:

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



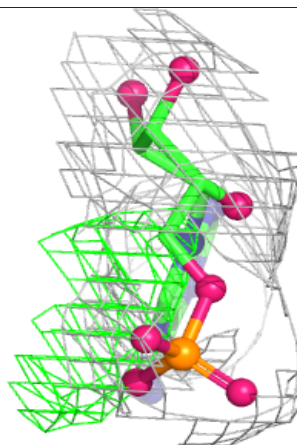
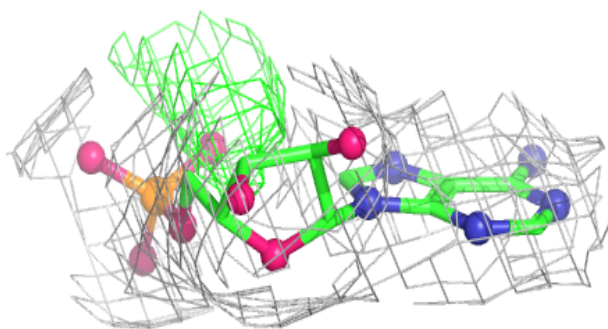
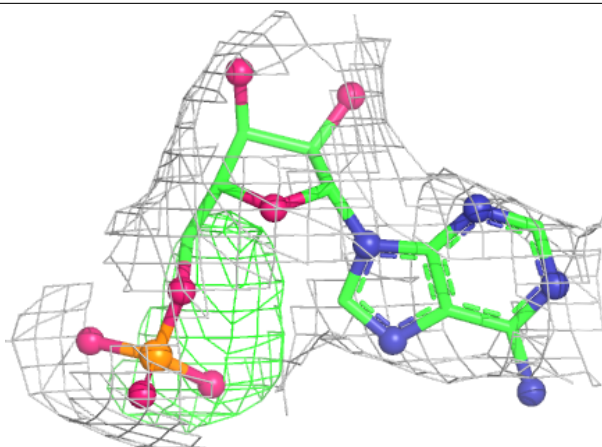
Electron density around AMP G 401:

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



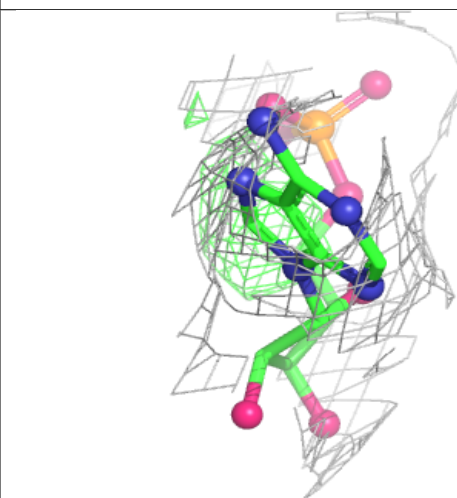
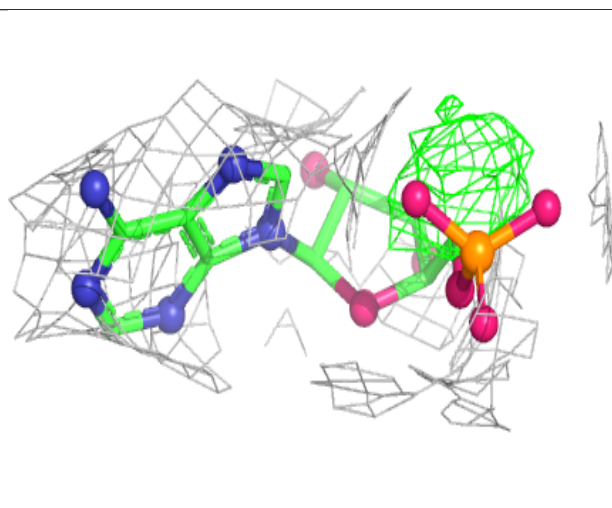
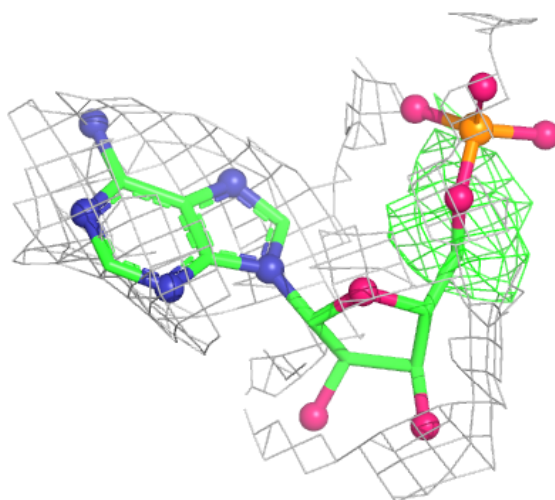
Electron density around AMP G 402:

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



Electron density around AMP G 403:

$2mF_o-DF_c$ (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.