Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 11:43 pm GMT

PDB ID	:	4CDD
Title	:	Human DPP1 in complex with (2S)-N-((1S)-1-cyano-2-(4-(4-cyanophenyl) phenyl)ethyl)piperidine-2-carboxamide
Authors	:	Debreczeni, J.; Edman, K.; Furber, M.; Tiden, A.; Gardiner, P.; Mete, T.; Ford, R.; Millichip, I.; Stein, L.; Mather, A.; Kinchin, E.; Luckhurst, C.; Cage, P.; Sanghanee, H.; Breed, J.; Wissler, L.
Deposited on	:	2013-10-31
Resolution	:	2.35 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 (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:

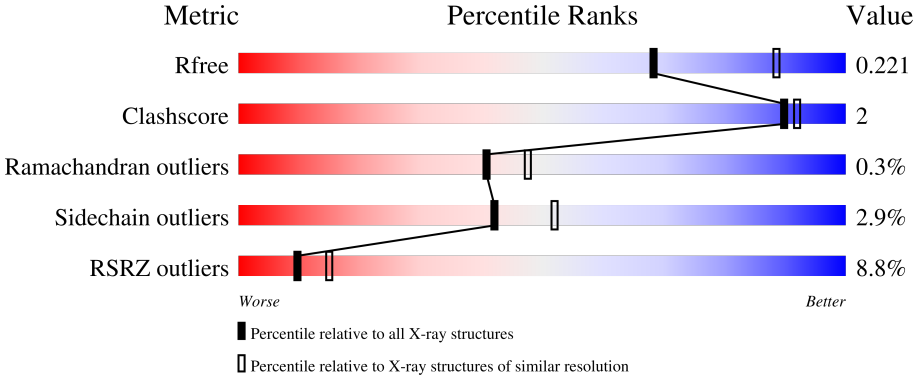
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	120	8% 92% 5% • •
1	D	120	17% 90% 6% •
2	B	165	4% 93% • • •
2	E	165	10% 89% 8% •
3	C	69	4% 96% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	69	9% 93%
4	G	2	100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5700 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 DIPEPTIDYL PEPTIDASE 1 EXCLUSION DOMAIN CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	118	946	608	153	179	6	0	0	0
1	D	115	920	593	149	172	6	0	0	0

- Molecule 2 is a protein called DIPEPTIDYL PEPTIDASE 1 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	162	1284	820	213	238	13	0	0	0
2	E	161	1274	814	210	237	13	0	0	0

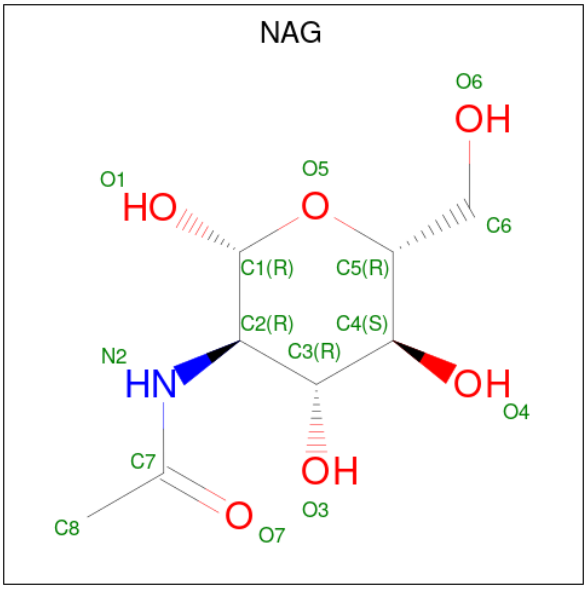
- Molecule 3 is a protein called DIPEPTIDYL PEPTIDASE 1 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	68	528	339	88	99	2	0	0	0
3	F	68	528	339	88	99	2	0	0	0

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

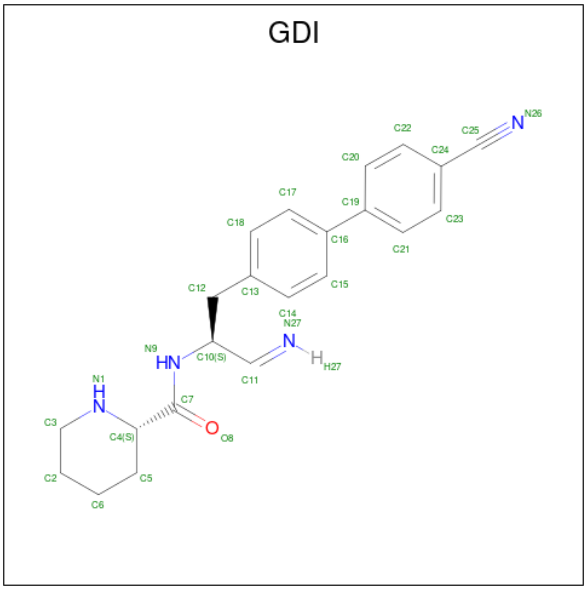
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	2	28	16	2	10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is (2S)-N-[(2S)-1-AZANYLIDENE-3-[4-(4-CYANOPHENYL)PHENYL]PROPAN-2-YL]PIPERIDINE-2-CARBOXAMIDE (three-letter code: GDI) (formula: $C_{22}H_{24}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	27	22	4	1	0	0
6	E	1	27	22	4	1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	B	1	1	1	0	0
7	E	1	1	1	0	0

- Molecule 8 is water.

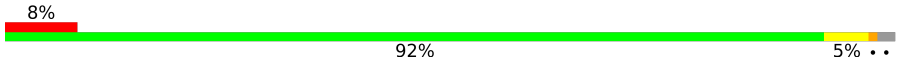
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	25	25	25	0	0
8	B	31	31	31	0	0
8	C	6	6	6	0	0
8	D	18	18	18	0	0
8	E	14	14	14	0	0

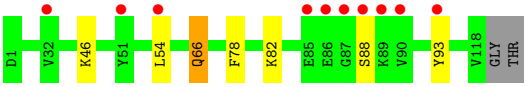
3 Residue-property plots (i)

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: DIPEPTIDYL PEPTIDASE 1 EXCLUSION DOMAIN CHAIN

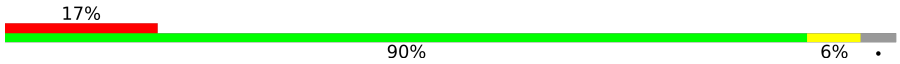
Chain A:

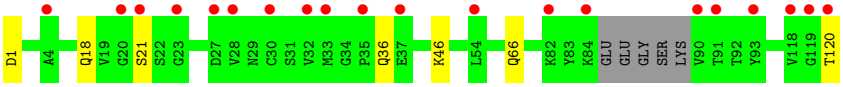




• Molecule 1: DIPEPTIDYL PEPTIDASE 1 EXCLUSION DOMAIN CHAIN

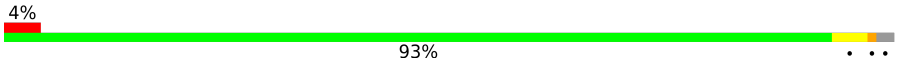
Chain D:

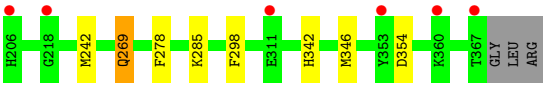




• Molecule 2: DIPEPTIDYL PEPTIDASE 1 HEAVY CHAIN

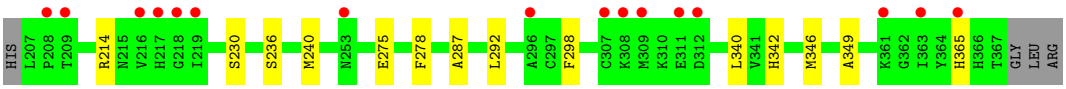
Chain B:





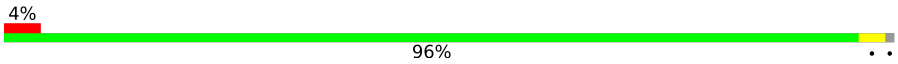
• Molecule 2: DIPEPTIDYL PEPTIDASE 1 HEAVY CHAIN

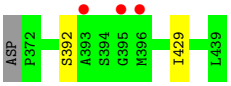
Chain E:



• Molecule 3: DIPEPTIDYL PEPTIDASE 1 LIGHT CHAIN

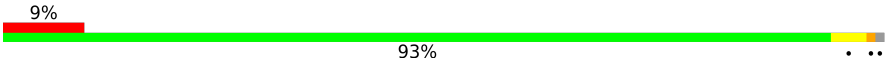
Chain C:

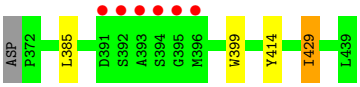




• Molecule 3: DIPEPTIDYL PEPTIDASE 1 LIGHT CHAIN

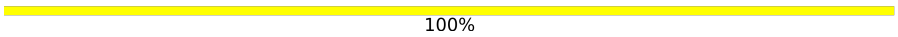
Chain F:





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

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	84.29Å 84.29Å 221.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.07 – 2.35 44.07 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.6 (44.07-2.35) 95.6 (44.07-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.187 , 0.223 0.190 , 0.221	Depositor DCC
R_{free} test set	1863 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	47.0	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5700	wwPDB-VP
Average B, all atoms (Å^2)	58.0	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDI, CL, NAG

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	0.45	0/971	0.60	0/1317
1	D	0.42	0/944	0.58	0/1281
2	B	0.42	0/1325	0.56	0/1796
2	E	0.39	0/1314	0.54	0/1781
3	C	0.42	0/544	0.61	0/740
3	F	0.40	0/544	0.58	0/740
All	All	0.42	0/5642	0.57	0/7655

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	946	0	897	3	0
1	D	920	0	875	4	0
2	B	1284	0	1185	5	0
2	E	1274	0	1178	10	0
3	C	528	0	502	0	0
3	F	528	0	502	4	0
4	G	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	E	14	0	13	0	0
6	B	27	0	22	1	0
6	E	27	0	22	1	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
8	A	25	0	0	0	0
8	B	31	0	0	0	0
8	C	6	0	0	0	0
8	D	18	0	0	0	0
8	E	14	0	0	0	0
All	All	5700	0	5247	19	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 2.

All (19) 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:E:278:PHE:CE2	6:E:1369:GDI:H31C	2.08	0.88
1:D:18:GLN:HG2	1:D:36:GLN:CD	2.09	0.74
1:D:66:GLN:HG3	2:E:278:PHE:CZ	2.35	0.61
1:A:66:GLN:HG3	2:B:278:PHE:CZ	2.37	0.59
1:D:66:GLN:HG3	2:E:278:PHE:CE1	2.41	0.56
2:E:236:SER:O	2:E:240:MET:HG2	2.06	0.56
1:D:18:GLN:HG2	1:D:36:GLN:NE2	2.26	0.49
2:B:242:MET:SD	2:B:346:MET:HA	2.54	0.48
2:E:349:ALA:HB3	3:F:429:ILE:CG2	2.45	0.47
2:E:287:ALA:HB2	2:E:292:LEU:HD11	1.99	0.45
3:F:385:LEU:HD11	3:F:399:TRP:CE3	2.52	0.45
2:E:340:LEU:HB2	2:E:346:MET:HE1	2.00	0.44
2:E:214:ARG:HD3	3:F:414:TYR:CZ	2.53	0.43
2:B:278:PHE:CE1	6:B:1369:GDI:H31C	2.54	0.43
2:E:275:GLU:CD	2:E:275:GLU:N	2.72	0.43
1:A:78:PHE:HB3	2:B:285:LYS:HE2	2.03	0.41
2:E:349:ALA:HB3	3:F:429:ILE:HG21	2.03	0.41
2:B:269:GLN:CD	2:B:269:GLN:H	2.24	0.40
1:A:82:LYS:HB3	1:A:93:TYR:HB2	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	116/120 (97%)	108 (93%)	8 (7%)	0	100	100
1	D	111/120 (92%)	104 (94%)	7 (6%)	0	100	100
2	B	160/165 (97%)	153 (96%)	7 (4%)	0	100	100
2	E	159/165 (96%)	150 (94%)	9 (6%)	0	100	100
3	C	66/69 (96%)	63 (96%)	2 (3%)	1 (2%)	10	8
3	F	66/69 (96%)	62 (94%)	3 (4%)	1 (2%)	10	8
All	All	678/708 (96%)	640 (94%)	36 (5%)	2 (0%)	41	47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	429	ILE
3	F	429	ILE

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	103/104 (99%)	99 (96%)	4 (4%)	32	40
1	D	100/104 (96%)	96 (96%)	4 (4%)	31	39
2	B	137/139 (99%)	133 (97%)	4 (3%)	42	52
2	E	136/139 (98%)	132 (97%)	4 (3%)	42	52
3	C	54/55 (98%)	53 (98%)	1 (2%)	57	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	54/55 (98%)	54 (100%)	0	100	100
All	All	584/596 (98%)	567 (97%)	17 (3%)	42	52

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LYS
1	A	54	LEU
1	A	66	GLN
1	A	88	SER
2	B	269	GLN
2	B	298	PHE
2	B	342	HIS
2	B	354	ASP
3	C	392	SER
1	D	1	ASP
1	D	21	SER
1	D	46	LYS
1	D	120	THR
2	E	230	SER
2	E	298	PHE
2	E	342	HIS
2	E	365	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	25	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

2 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	NAG	G	1	1,4	14,14,15	0.51	0	17,19,21	1.38	3 (17%)
4	NAG	G	2	4	14,14,15	0.51	0	17,19,21	1.31	2 (11%)

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	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1	NAG	C8-C7-N2	3.63	122.24	116.10
4	G	2	NAG	C8-C7-N2	2.76	120.78	116.10
4	G	1	NAG	C2-N2-C7	2.74	126.80	122.90
4	G	2	NAG	C1-C2-N2	-2.41	106.37	110.49
4	G	1	NAG	O7-C7-C8	-2.25	117.87	122.06

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

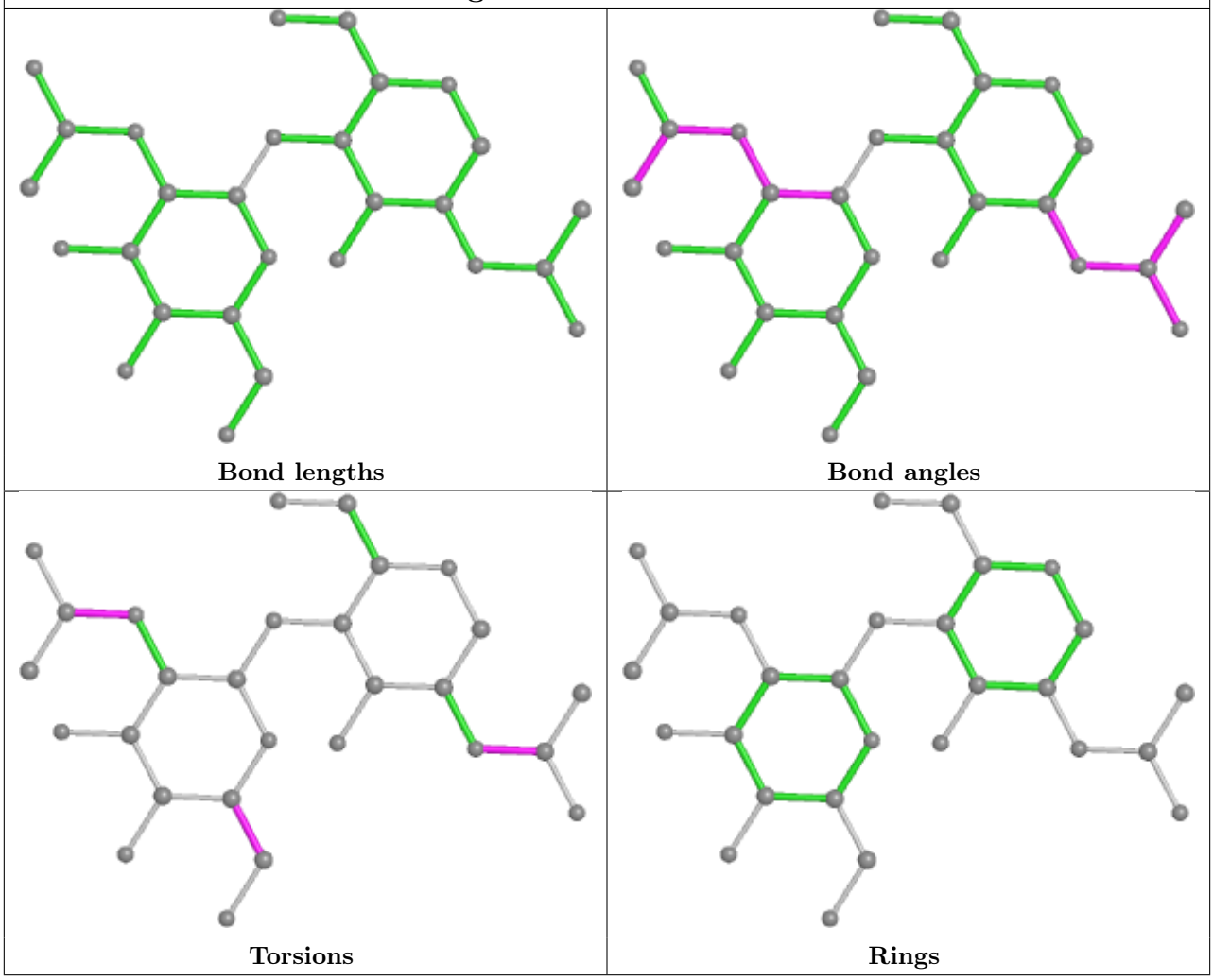
Mol	Chain	Res	Type	Atoms
4	G	2	NAG	O7-C7-N2-C2
4	G	2	NAG	O5-C5-C6-O6

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.

Oligosaccharide Chain G



5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	1119	1	14,14,15	0.55	0	17,19,21	1.22	2 (11%)
6	GDI	E	1369	2	27,29,29	0.57	0	32,38,38	1.11	3 (9%)
5	NAG	B	1368	2	14,14,15	0.56	0	17,19,21	1.29	2 (11%)
5	NAG	E	1368	2	14,14,15	0.52	0	17,19,21	1.78	4 (23%)
6	GDI	B	1369	2	27,29,29	0.66	0	32,38,38	1.24	2 (6%)

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	NAG	A	1119	1	-	4/6/23/26	0/1/1/1
6	GDI	E	1369	2	-	3/18/28/28	0/3/3/3
5	NAG	B	1368	2	-	0/6/23/26	0/1/1/1
5	NAG	E	1368	2	-	4/6/23/26	0/1/1/1
6	GDI	B	1369	2	-	0/18/28/28	0/3/3/3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1368	NAG	O5-C1-C2	-4.68	103.90	111.29
6	B	1369	GDI	C6-C5-C4	-3.70	105.95	111.04
6	B	1369	GDI	C13-C12-C10	-3.23	109.01	113.63
5	B	1368	NAG	O5-C5-C6	3.21	112.24	107.20
5	E	1368	NAG	C1-O5-C5	3.10	116.39	112.19
5	E	1368	NAG	C8-C7-N2	2.86	120.94	116.10
5	A	1119	NAG	C1-C2-N2	2.63	114.97	110.49
5	B	1368	NAG	C1-C2-N2	-2.59	106.06	110.49
6	E	1369	GDI	C20-C19-C16	-2.29	117.39	121.36
6	E	1369	GDI	C11-C10-N9	-2.27	106.37	110.54
6	E	1369	GDI	C13-C12-C10	-2.25	110.42	113.63
5	A	1119	NAG	C2-N2-C7	2.23	126.08	122.90
5	E	1368	NAG	C1-C2-N2	2.10	114.08	110.49

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1119	NAG	C4-C5-C6-O6
5	A	1119	NAG	O5-C5-C6-O6
5	E	1368	NAG	O5-C5-C6-O6
5	E	1368	NAG	C8-C7-N2-C2
5	E	1368	NAG	O7-C7-N2-C2
5	E	1368	NAG	C4-C5-C6-O6
5	A	1119	NAG	C1-C2-N2-C7
6	E	1369	GDI	C5-C4-C7-O8
6	E	1369	GDI	C5-C4-C7-N9
6	E	1369	GDI	N1-C4-C7-N9
5	A	1119	NAG	C3-C2-N2-C7

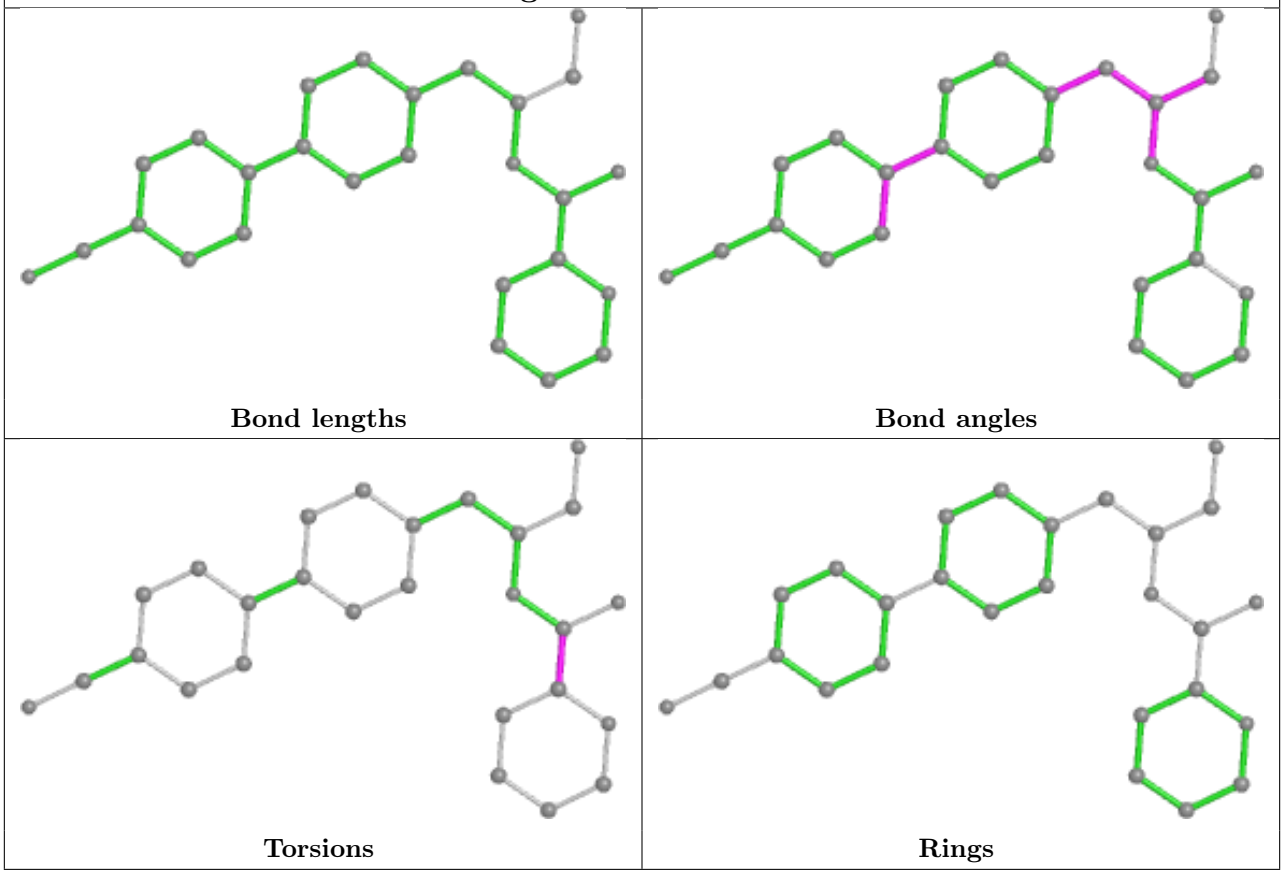
There are no ring outliers.

2 monomers are involved in 2 short contacts:

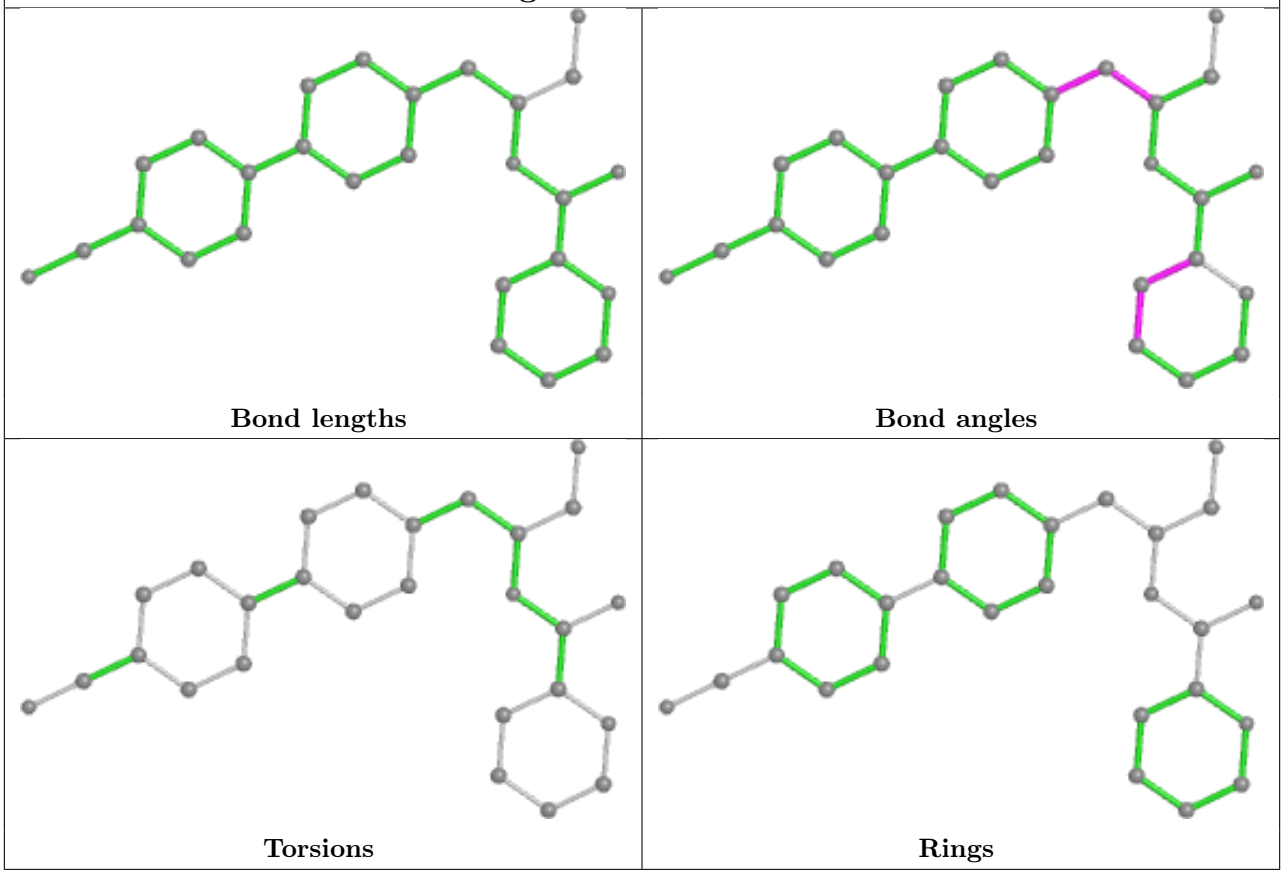
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1369	GDI	1	0
6	B	1369	GDI	1	0

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 GDI E 1369



Ligand GDI B 1369



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	118/120 (98%)	0.45	10 (8%) 10 16	33, 51, 84, 124	0
1	D	115/120 (95%)	0.98	20 (17%) 1 2	35, 57, 103, 120	0
2	B	162/165 (98%)	0.23	6 (3%) 41 54	33, 49, 77, 90	0
2	E	161/165 (97%)	0.42	16 (9%) 7 11	36, 62, 94, 107	0
3	C	68/69 (98%)	0.27	3 (4%) 34 46	35, 51, 79, 94	0
3	F	68/69 (98%)	0.28	6 (8%) 10 15	37, 64, 98, 119	0
All	All	692/708 (97%)	0.44	61 (8%) 10 15	33, 55, 92, 124	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	119	GLY	8.2
1	D	93	TYR	6.9
1	A	86	GLU	6.8
1	D	120	THR	6.6
1	D	32	VAL	5.5
1	D	33	MET	5.3
2	E	308	LYS	4.9
3	F	393	ALA	4.9
3	C	395	GLY	4.8
1	D	23	GLY	4.6
1	A	85	GLU	4.2
1	A	89	LYS	3.9
1	D	21	SER	3.9
1	D	91	THR	3.9
1	D	37	GLU	3.8
1	A	88	SER	3.8
2	E	217	HIS	3.7
2	B	311	GLU	3.7
1	A	32	VAL	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	363	ILE	3.4
1	A	54	LEU	3.4
3	F	394	SER	3.4
2	E	311	GLU	3.4
1	D	4	ALA	3.3
3	C	396	MET	3.2
1	D	35	PRO	3.2
2	B	218	GLY	3.0
1	A	87	GLY	3.0
2	E	208	PRO	2.9
1	D	27	ASP	2.9
1	A	93	TYR	2.9
1	D	90	VAL	2.9
2	E	216	VAL	2.8
1	D	54	LEU	2.8
3	F	395	GLY	2.6
2	B	206	HIS	2.6
2	E	309	MET	2.5
2	E	312	ASP	2.5
2	E	296	ALA	2.5
1	D	28	VAL	2.5
1	D	84	LYS	2.5
1	D	118	VAL	2.4
2	B	367	THR	2.4
2	B	353	TYR	2.4
2	E	209	THR	2.4
3	F	391	ASP	2.3
1	D	82	LYS	2.3
1	D	30	CYS	2.2
2	E	218	GLY	2.2
2	E	365	HIS	2.2
2	E	307	CYS	2.2
3	F	392	SER	2.2
1	A	90	VAL	2.2
2	E	253	ASN	2.1
2	B	360	LYS	2.1
2	E	361	LYS	2.1
2	E	219	ILE	2.1
1	D	20	GLY	2.0
3	C	393	ALA	2.0
1	A	51	TYR	2.0
3	F	396	MET	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

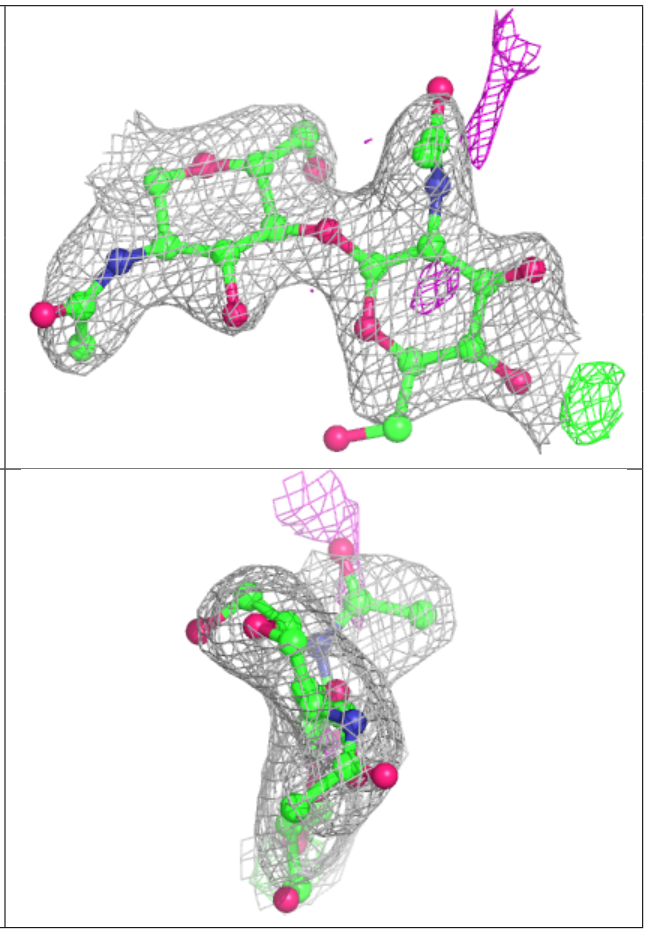
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	G	2	14/15	0.81	0.38	64,84,97,99	0
4	NAG	G	1	14/15	0.91	0.29	63,76,82,87	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 G:

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 (i)

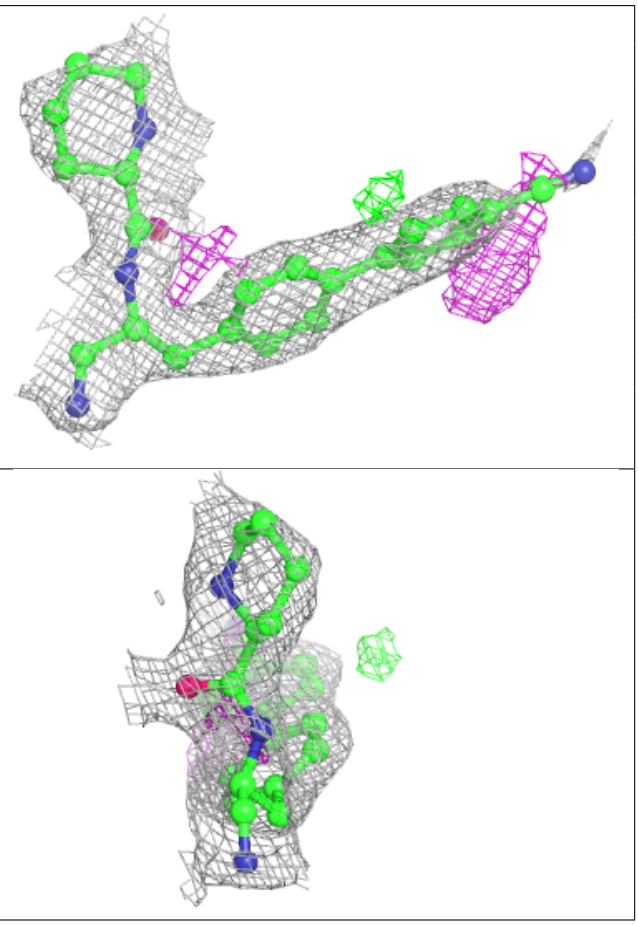
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	A	1119	14/15	0.80	0.39	95,110,115,118	0
5	NAG	B	1368	14/15	0.87	0.24	62,77,88,97	0
6	GDI	E	1369	27/27	0.88	0.19	53,60,65,74	0
6	GDI	B	1369	27/27	0.91	0.15	38,49,52,57	0
5	NAG	E	1368	14/15	0.91	0.22	78,90,99,100	0
7	CL	E	1370	1/1	0.97	0.17	46,46,46,46	0
7	CL	B	1370	1/1	0.99	0.20	43,43,43,43	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.

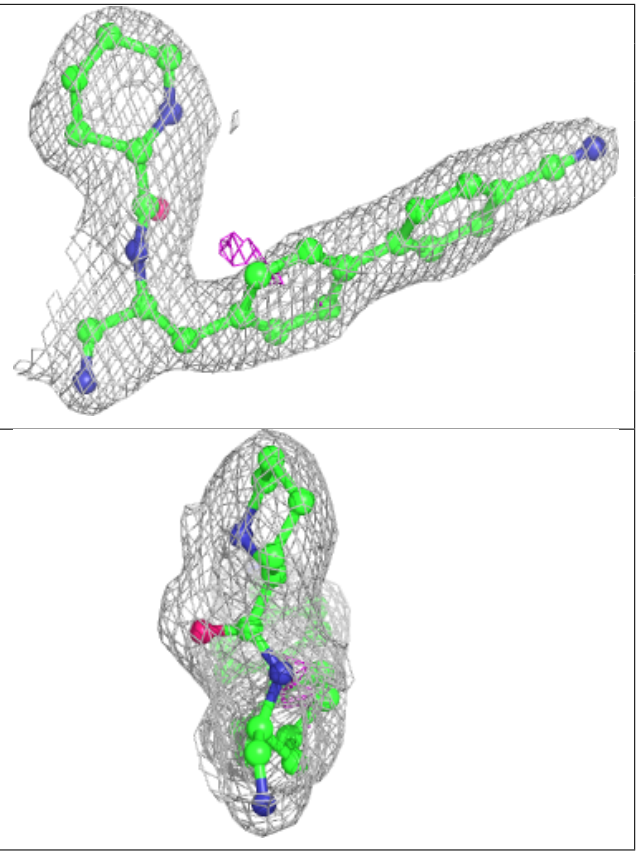
Electron density around GDI E 1369:

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 GDI B 1369:

$2mF_o$-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.