Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID	:	8QCE
Title	:	Dispersin from Lactiplantibacillus paraplantarum DispLp
Authors	:	Males, A.; Moroz, O.V.; Blagova, E.; Munch, A.; Hansen, G.H.; Johansen, A.H.; Ostergaard, L.H.; Segura, D.R.; Eddenden, A.; Due, A.V.; Gudmand, M.; Salomon, J.; Sorensen, S.R.; Cairo, J.L.F.; Pache, R.A.; Vejborg, R.M.; Davies, G.J.; Wilson, K.S.
Deposited on	:	2023-08-25
Resolution	:	1.05 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 (1)) were used in the production of this report:

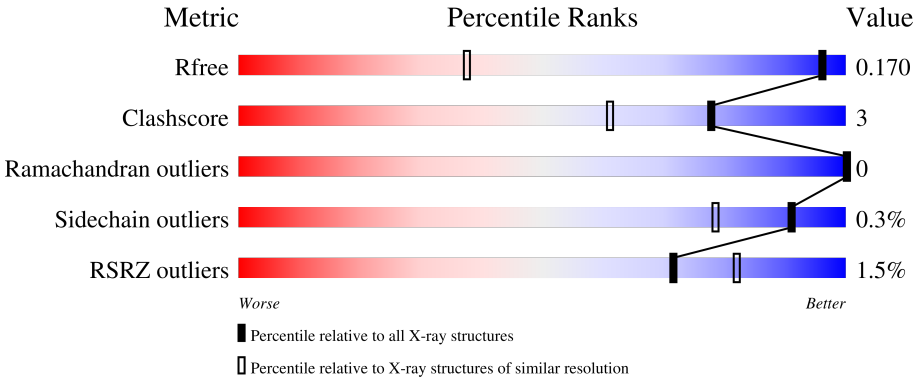
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 1.05 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}	164625	1027 (1.08-1.04)
Clashscore	180529	1152 (1.08-1.04)
Ramachandran outliers	177936	1127 (1.08-1.04)
Sidechain outliers	177891	1128 (1.08-1.04)
RSRZ outliers	164620	1026 (1.08-1.04)

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

Mol	Chain	Length	Quality of chain
1	A	336	93% 6%
1	B	336	93% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	B	403	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11788 atoms, of which 5405 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called N-acetyl-beta-hexosaminidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	333	Total	C	H	N	O	S	105	13	0
			5318	1691	2614	460	546	7			
1	B	336	Total	C	H	N	O	S	105	26	0
			5583	1787	2727	492	571	6			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	expression tag	UNP A0A370AE65
A	-3	HIS	-	expression tag	UNP A0A370AE65
A	-2	HIS	-	expression tag	UNP A0A370AE65
A	-1	PRO	-	expression tag	UNP A0A370AE65
A	0	ARG	-	expression tag	UNP A0A370AE65
A	45	SER	ALA	conflict	UNP A0A370AE65
A	60	ALA	THR	conflict	UNP A0A370AE65
A	79	ASN	ASP	conflict	UNP A0A370AE65
A	128	ILE	VAL	conflict	UNP A0A370AE65
A	181	HIS	ASN	conflict	UNP A0A370AE65
A	198	THR	ASN	conflict	UNP A0A370AE65
A	218	VAL	ALA	conflict	UNP A0A370AE65
A	229	VAL	ALA	conflict	UNP A0A370AE65
B	-4	HIS	-	expression tag	UNP A0A370AE65
B	-3	HIS	-	expression tag	UNP A0A370AE65
B	-2	HIS	-	expression tag	UNP A0A370AE65
B	-1	PRO	-	expression tag	UNP A0A370AE65
B	0	ARG	-	expression tag	UNP A0A370AE65
B	45	SER	ALA	conflict	UNP A0A370AE65
B	60	ALA	THR	conflict	UNP A0A370AE65
B	79	ASN	ASP	conflict	UNP A0A370AE65
B	128	ILE	VAL	conflict	UNP A0A370AE65
B	181	HIS	ASN	conflict	UNP A0A370AE65
B	198	THR	ASN	conflict	UNP A0A370AE65
B	218	VAL	ALA	conflict	UNP A0A370AE65

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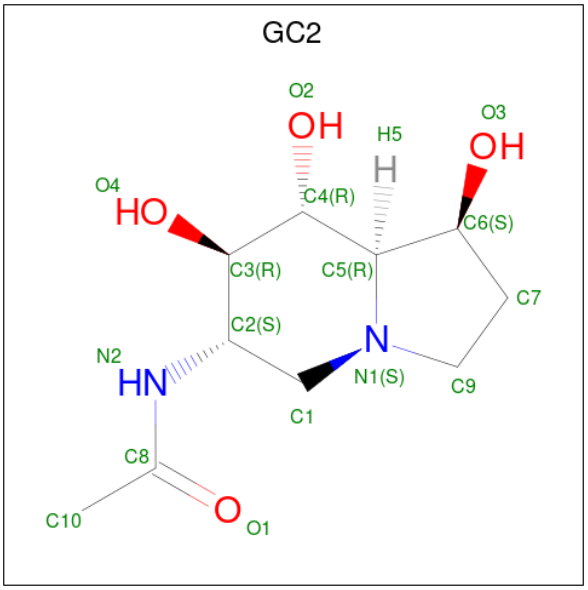
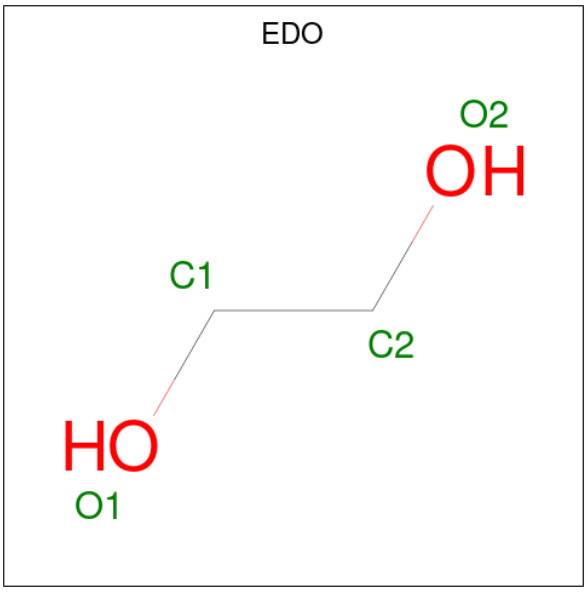
Chain	Residue	Modelled	Actual	Comment	Reference
B	229	VAL	ALA	conflict	UNP A0A370AE65

- Molecule 2 is 6-ACETAMIDO-6-DEOXY-CASTANOSPERMINE (three-letter code: GC2) (formula: $C_{10}H_{18}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



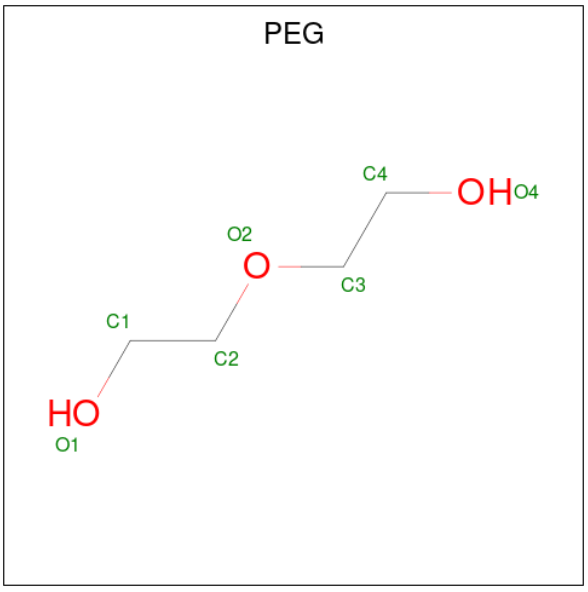
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	3	0
			34	10	18	2	4		
2	B	1	Total	C	H	N	O	3	0
			34	10	18	2	4		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	1	0
			10	2	6	2		
3	A	1	Total	C	H	O	1	0
			10	2	6	2		
3	B	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	1	0
			17	4	10	3		

- Molecule 5 is water.

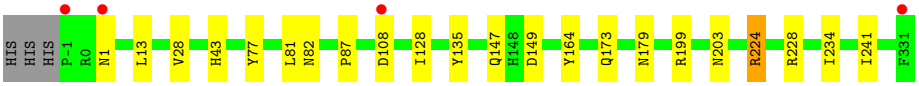
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	419	Total O 419 419	0	0
5	B	353	Total O 353 353	0	0

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.

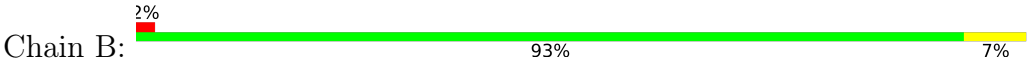
• Molecule 1: N-acetyl-beta-hexosaminidase

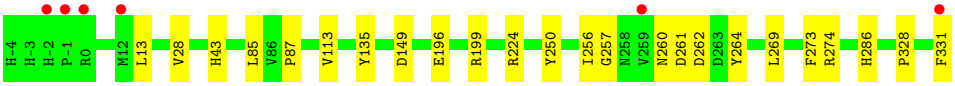
Chain A:



• Molecule 1: N-acetyl-beta-hexosaminidase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.90Å 82.79Å 80.64Å 90.00° 98.11° 90.00°	Depositor
Resolution (Å)	38.06 – 1.05 38.06 – 1.05	Depositor EDS
% Data completeness (in resolution range)	90.5 (38.06-1.05) 90.5 (38.06-1.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 1.05Å)	Xtriage
Refinement program	REFMAC 5.8.0419, REFMAC 5.8.0419	Depositor
R, R_{free}	0.147 , 0.170 0.147 , 0.170	Depositor DCC
R_{free} test set	12701 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	10.4	Xtriage
Anisotropy	0.728	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	11788	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PEG, GC2

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	0.64	1/2759 (0.0%)	0.88	6/3769 (0.2%)
1	B	0.55	0/2920	0.85	5/3993 (0.1%)
All	All	0.59	1/5679 (0.0%)	0.86	11/7762 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	ASP	CG-OD1	5.20	1.37	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ASP	CB-CG-OD1	7.67	125.20	118.30
1	B	224	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	224	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	135	TYR	CB-CG-CD1	6.20	124.72	121.00
1	B	85	LEU	CB-CG-CD2	6.14	121.44	111.00
1	A	164	TYR	CB-CG-CD1	5.74	124.44	121.00
1	B	135	TYR	CB-CG-CD1	5.70	124.42	121.00
1	A	108	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	B	331	PHE	CB-CG-CD2	-5.33	117.07	120.80
1	A	228	ARG	NE-CZ-NH2	-5.19	117.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	250	TYR	CB-CG-CD1	5.11	124.06	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Sidechain

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	2704	2614	2581	14	0
1	B	2856	2727	2706	18	0
2	A	16	18	18	0	0
2	B	16	18	18	0	0
3	A	8	12	12	0	0
3	B	4	6	6	0	0
4	B	7	10	10	8	0
5	A	419	0	0	2	1
5	B	353	0	0	2	0
All	All	6383	5405	5351	30	1

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 3.

All (30) 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:B:264[B]:TYR:OH	4:B:403:PEG:H12	1.65	0.97
1:B:257[A]:GLY:N	1:B:262[A]:ASP:OD2	2.16	0.74
1:A:81:LEU:O	4:B:403:PEG:H31	1.88	0.72
1:B:264[B]:TYR:OH	4:B:403:PEG:C1	2.38	0.71
1:B:257[A]:GLY:H	1:B:262[A]:ASP:CG	2.00	0.64
1:B:256[A]:ILE:HA	1:B:262[A]:ASP:OD1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13[B]:LEU:HD21	1:A:28:VAL:HG21	1.81	0.62
1:A:128:ILE:HD13	1:A:173:GLN:OE1	2.00	0.61
1:B:269[B]:LEU:O	1:B:328:PRO:HD3	2.00	0.61
1:B:260[B]:ASN:CG	5:B:503:HOH:O	2.44	0.56
1:A:43:HIS:CE1	5:A:504:HOH:O	2.59	0.55
1:B:196:GLU:OE1	1:B:199:ARG:NH2	2.41	0.54
1:B:264[B]:TYR:HE1	4:B:403:PEG:HO1	1.53	0.52
1:A:234:ILE:HG21	1:A:241[B]:ILE:HG12	1.92	0.52
1:A:13[A]:LEU:HD11	1:A:28:VAL:HG11	1.95	0.49
1:A:128:ILE:HD13	1:A:173:GLN:CD	2.33	0.48
1:B:264[A]:TYR:OH	4:B:403:PEG:H12	2.12	0.48
1:B:87:PRO:HD2	1:B:149:ASP:O	2.15	0.47
1:A:199:ARG:HG3	5:A:534:HOH:O	2.14	0.46
1:A:1:ASN:HB2	1:A:203:ASN:HB2	1.97	0.45
1:A:13[B]:LEU:CD2	1:A:28:VAL:HG21	2.47	0.44
1:B:264[B]:TYR:CE1	4:B:403:PEG:O1	2.70	0.44
1:B:264[B]:TYR:HE1	4:B:403:PEG:O1	2.00	0.43
1:B:43:HIS:CE1	5:B:517:HOH:O	2.71	0.43
1:B:13:LEU:HD11	1:B:28:VAL:HG11	2.00	0.43
1:A:77:TYR:OH	1:B:261[B]:ASP:OD1	2.37	0.42
1:A:82:ASN:HB3	4:B:403:PEG:H42	2.02	0.41
1:B:273[B]:PHE:O	1:B:274[B]:ARG:HD3	2.21	0.41
1:A:147[B]:GLN:OE1	1:B:286:HIS:CD2	2.74	0.41
1:A:87:PRO:HD2	1:A:149:ASP:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:559:HOH:O	5:A:837:HOH:O[1_455]	2.04	0.16

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	344/336 (102%)	340 (99%)	4 (1%)	0	100	100
1	B	360/336 (107%)	353 (98%)	7 (2%)	0	100	100
All	All	704/672 (105%)	693 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	302/293 (103%)	301 (100%)	1 (0%)	91	78
1	B	318/293 (108%)	316 (99%)	2 (1%)	84	63
All	All	620/586 (106%)	617 (100%)	3 (0%)	91	67

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	B	113[A]	VAL
1	B	113[B]	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	184	ASN
1	B	111	ASN

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)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GC2	B	401	-	16,17,17	0.87	0	17,25,25	1.45	3 (17%)
2	GC2	A	401	-	16,17,17	0.85	0	17,25,25	1.14	3 (17%)
3	EDO	A	403	-	3,3,3	0.67	0	2,2,2	1.25	0
4	PEG	B	403	-	6,6,6	0.21	0	5,5,5	0.58	0
3	EDO	B	402	-	3,3,3	0.19	0	2,2,2	0.48	0
3	EDO	A	402	-	3,3,3	0.43	0	2,2,2	0.15	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	GC2	B	401	-	-	4/4/33/33	1/2/2/2
2	GC2	A	401	-	-	1/4/33/33	1/2/2/2
3	EDO	A	403	-	-	0/1/1/1	-
4	PEG	B	403	-	-	2/4/4/4	-
3	EDO	B	402	-	-	0/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	GC2	O4-C3-C4	-4.33	100.34	110.35
2	A	401	GC2	O4-C3-C2	2.66	114.97	109.47
2	A	401	GC2	O4-C3-C4	-2.23	105.20	110.35
2	B	401	GC2	O4-C3-C2	2.19	113.99	109.47
2	A	401	GC2	C1-C2-N2	2.13	112.78	109.71
2	B	401	GC2	C9-C7-C6	-2.11	100.44	103.74

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	403	PEG	O1-C1-C2-O2
2	B	401	GC2	C10-C8-N2-C2
2	A	401	GC2	C1-C2-N2-C8
4	B	403	PEG	C4-C3-O2-C2
2	B	401	GC2	C1-C2-N2-C8
2	B	401	GC2	O1-C8-N2-C2
2	B	401	GC2	C3-C2-N2-C8

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	GC2	C1-C2-C3-C4-C5-N1
2	A	401	GC2	C1-C2-C3-C4-C5-N1

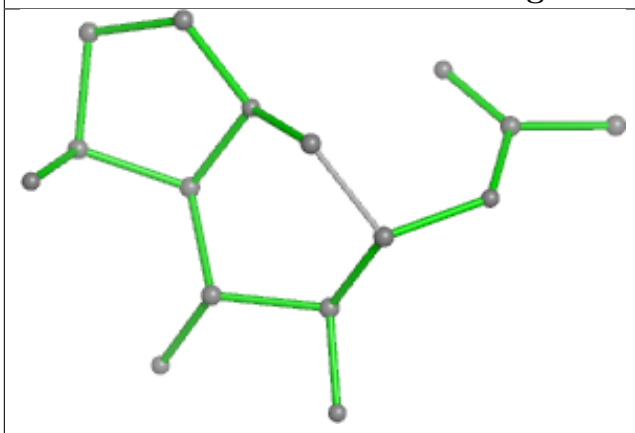
1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	403	PEG	8	0

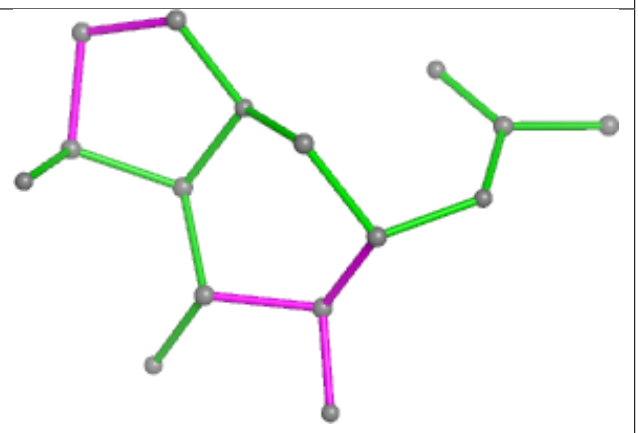
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

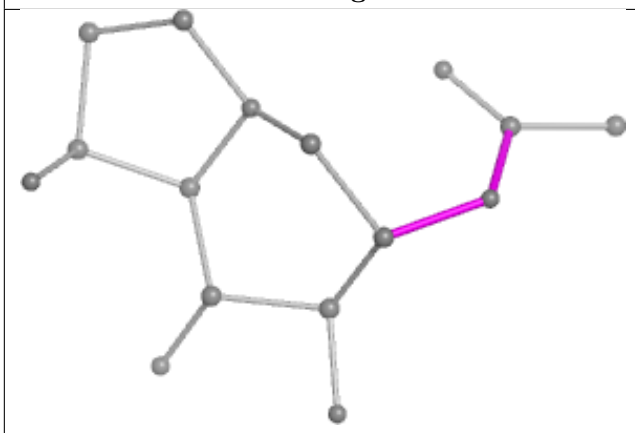
Ligand GC2 B 401



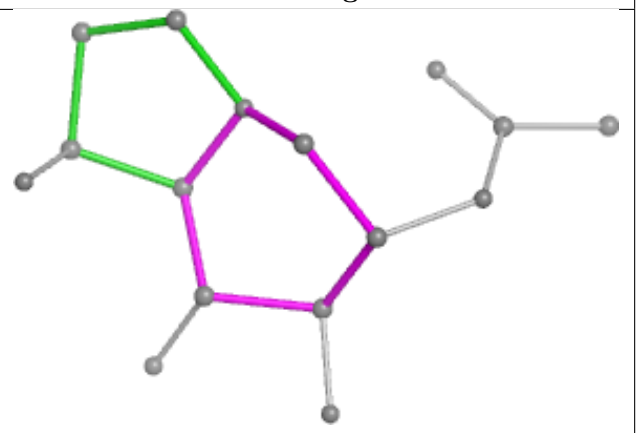
Bond lengths



Bond angles

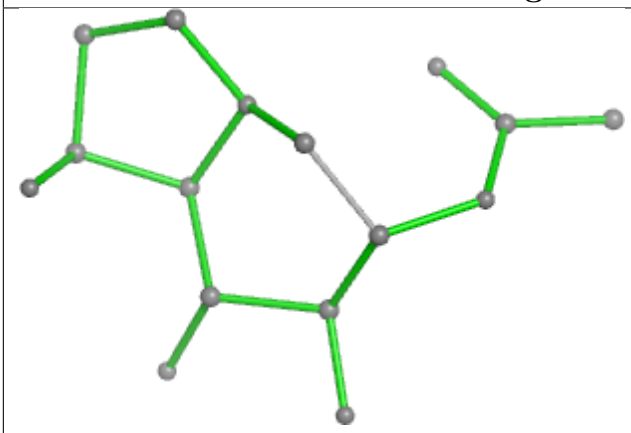


Torsions

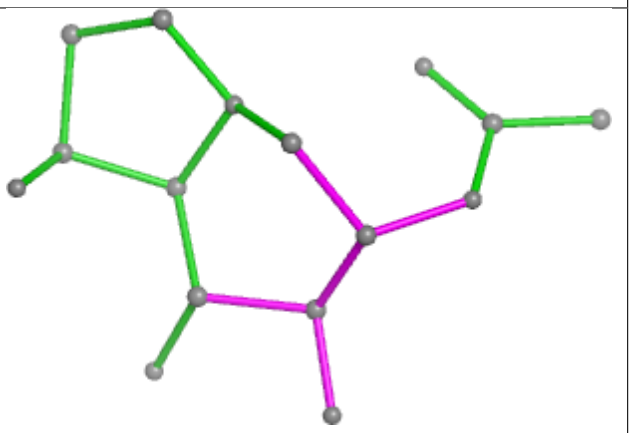


Rings

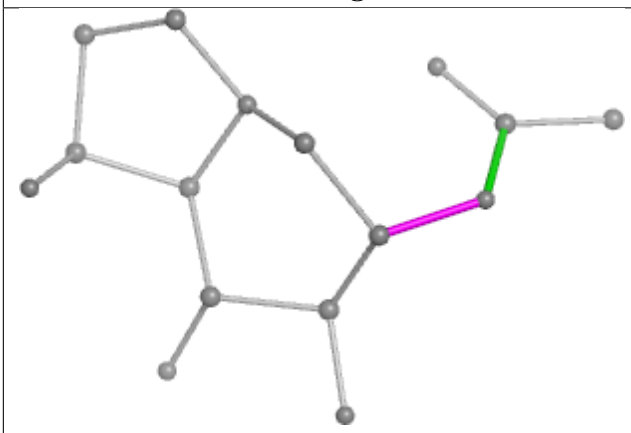
Ligand GC2 A 401



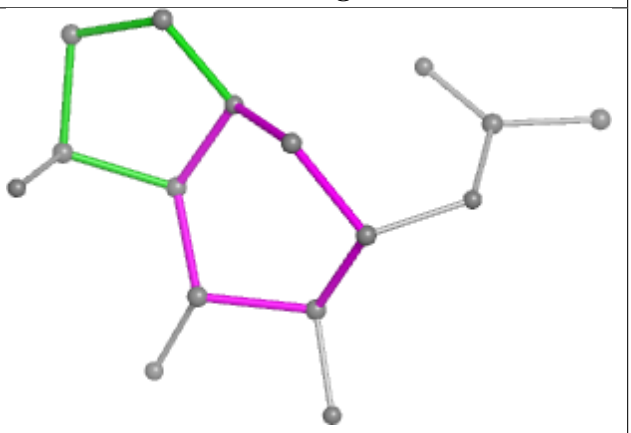
Bond lengths



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	333/336 (99%)	-0.39	4 (1%)	76	86	5, 11, 21, 34	13 (3%)
1	B	336/336 (100%)	-0.07	6 (1%)	67	78	6, 14, 26, 92	26 (7%)
All	All	669/672 (99%)	-0.23	10 (1%)	71	82	5, 12, 25, 92	39 (5%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-1	PRO	4.2
1	A	1	ASN	3.4
1	B	-2	HIS	3.2
1	A	108	ASP	3.1
1	B	331	PHE	2.6
1	B	12	MET	2.6
1	B	259[A]	VAL	2.4
1	A	331	PHE	2.3
1	A	-1	PRO	2.2
1	B	0	ARG	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

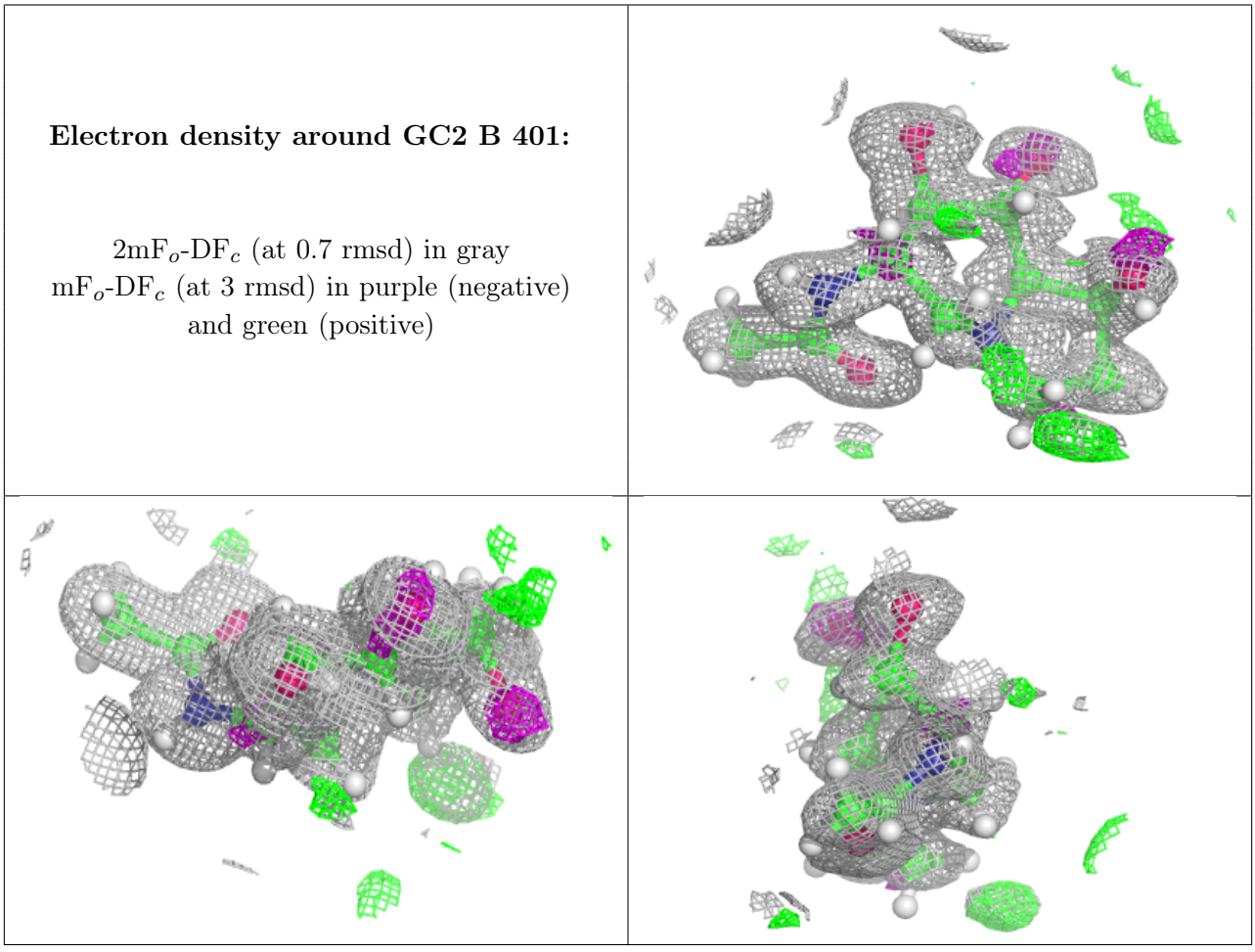
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PEG	B	403	7/7	0.62	0.37	32,35,42,44	17
3	EDO	A	403	4/4	0.95	0.09	11,18,19,19	1
3	EDO	B	402	4/4	0.96	0.08	14,19,21,22	1
3	EDO	A	402	4/4	0.96	0.07	19,19,23,23	1
2	GC2	B	401	16/16	0.97	0.07	9,16,19,23	3
2	GC2	A	401	16/16	0.98	0.06	10,14,17,20	3

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.

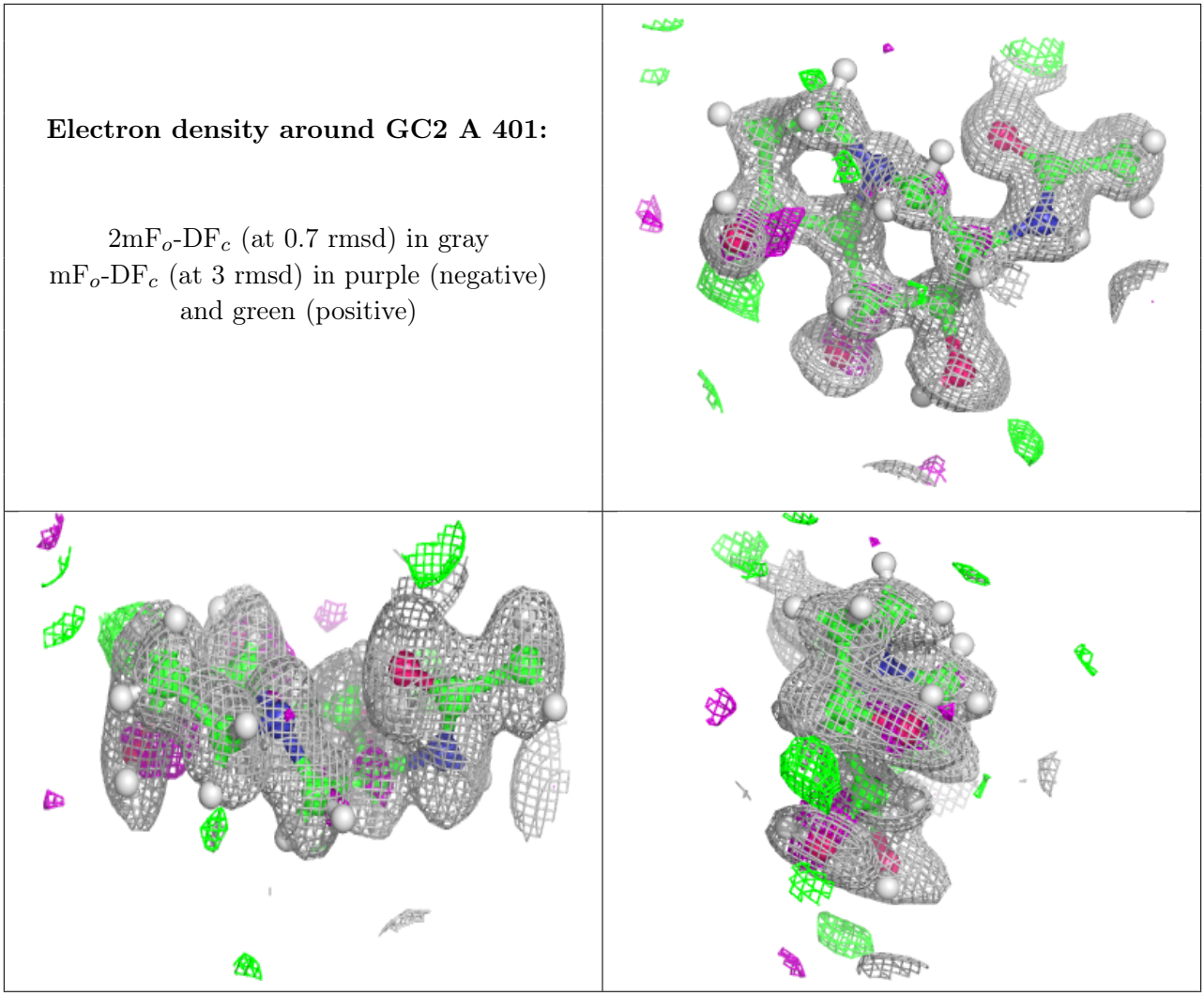
Electron density around GC2 B 401:

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



Electron density around GC2 A 401:

$2mF_o$-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

There are no such residues in this entry.