



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:14 AM UTC

PDB ID : 8OM0 / pdb_00008om0
Title : Structure of Oceanobacillus iheyensis group II intron in the presence of Na⁺, Mg²⁺ and intronistat B
Authors : Silvestri, I.; Marcia, M.
Deposited on : 2023-03-31
Resolution : 3.61 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

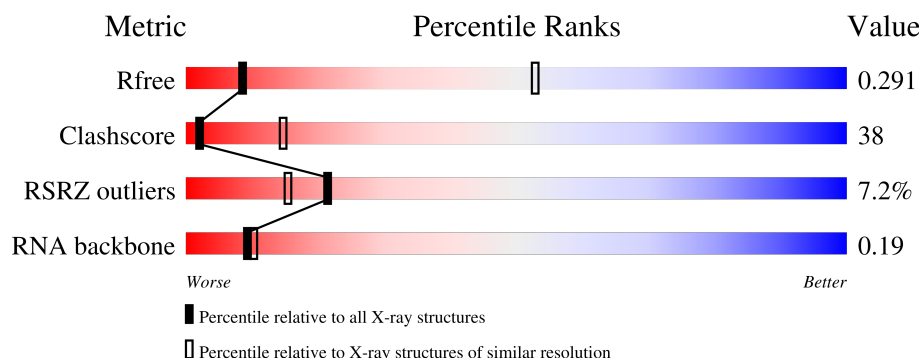
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.61 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	1062 (3.72-3.52)
Clashscore	190562	1092 (3.72-3.52)
RSRZ outliers	180081	1060 (3.72-3.52)
RNA backbone	3983	1018 (4.18-3.06)

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	394	7% 9% 33% 39% 18%

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
2	GDE	A	401	-	X	-	-

2 Entry composition [i](#)

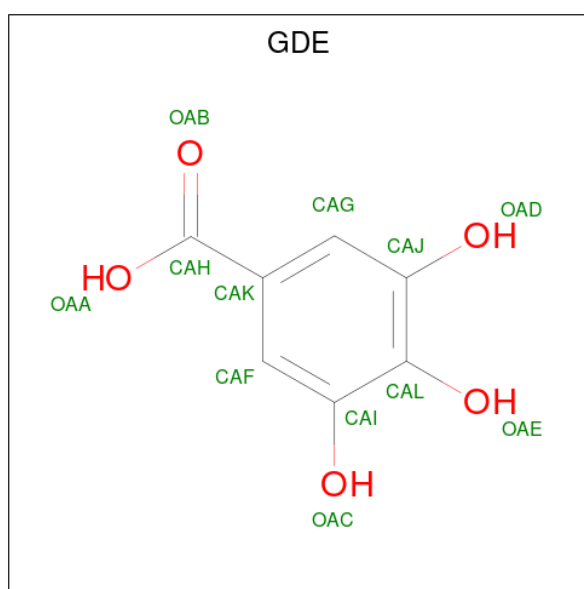
There are 4 unique types of molecules in this entry. The entry contains 8375 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RNA chain called Domains 1-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	390	8349	3725	1541	2693	390	0	0	0

- Molecule 2 is 3,4,5-trihydroxybenzoic acid (CCD ID: GDE) (formula: $C_7H_6O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	Mg	0	0
			10	10		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total 5	Na 5	0	0

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.

Chain A:

7% 9% 33% 39% 18%

Category	Value
G	658
G	659
G	660
G	661
U2	662
G3	663
U4	664
G5	665
C6	666
C7	667
G8	668
C9	669
G10	670
C11	671
A12	672
U13	673
G14	674
G15	675
G16	676
U17	677
G18	678
C19	679
G20	680
A21	681
G22	682
C23	683
U24	684
A25	685
G26	686
A27	687
G28	688
C29	689
G30	690
U31	691
G32	692
A33	693
G34	694
A35	695
G36	696
U37	697
C38	698
C39	699
C40	700
G41	701
A42	702
A43	703
C44	704
U45	705
G46	706
U47	707
G48	708
A49	709
A50	710
G51	711
C52	712
C53	713
A54	714
G55	715
A56	716
C57	717
A58	718
G59	719
C60	720
A61	721
G62	722
C63	723
A64	724
G65	725
C66	726
A67	727
G68	728
C69	729
A70	730
G71	731
C72	732
A73	733
G74	734
C75	735
A76	736
G77	737
C78	738
A79	739
G80	740
C81	741
A82	742
G83	743
C84	744
A85	745
G86	746
C87	747
A88	748
G89	749
C90	750
A91	751
G92	752
C93	753
A94	754
G95	755
C96	756
A97	757
G98	758
C99	759
A100	760
G101	761
C102	762
A103	763
G104	764
C105	765
A106	766
G107	767
C108	768
A109	769
G110	770
C111	771
A112	772
G113	773
C114	774
A115	775
G116	776
C117	777
A118	778
G119	779
C120	780
A121	781
G122	782
C123	783
A124	784
G125	785
C126	786
A127	787
G128	788
C129	789
A130	790
G131	791
C132	792
A133	793
G134	794
C135	795
A136	796
G137	797
C138	798
A139	799
G140	800
C141	801
A142	802
G143	803
C144	804
A145	805
G146	806
C147	807
A148	808
G149	809
C150	810
A151	811
G152	812
C153	813
A154	814
G155	815
C156	816
A157	817
G158	818
C159	819
A160	820
G161	821
C162	822
A163	823
G164	824
C165	825
A166	826
G167	827
C168	828
A169	829
G170	830
C171	831
A172	832
G173	833
C174	834
A175	835
G176	836
C177	837
A178	838
G179	839
C180	840
A181	841
C182	842
A184	843
G187	844
A188	845
C189	846
A190	847
G191	848
C192	849
A193	850
G194	851
C195	852
A196	853
G197	854
C198	855
A199	856
G200	857
C201	858
A202	859
G203	860
C204	8

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.81Å 94.28Å 223.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.35 – 3.61 47.35 – 3.61	Depositor EDS
% Data completeness (in resolution range)	96.8 (47.35-3.61) 96.9 (47.35-3.61)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.238 , 0.296 0.238 , 0.291	Depositor DCC
R_{free} test set	1082 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	202.1	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 144.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8375	wwPDB-VP
Average B, all atoms (Å ²)	225.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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: NA, GDE, MG

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	0.74	1/9355 (0.0%)	1.50	232/14593 (1.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	A	C3'-O3'	6.20	1.51	1.42

The worst 5 of 232 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	G	P-O3'-C3'	-16.05	96.13	120.20
1	A	170	G	P-O3'-C3'	-12.99	100.71	120.20
1	A	117	G	P-O3'-C3'	-12.37	101.64	120.20
1	A	57	A	C2'-C3'-O3'	-12.33	95.20	113.70
1	A	54	A	P-O3'-C3'	-12.26	101.82	120.20

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	8349	0	4192	466	1
2	A	11	0	2	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	0	0	0
4	A	5	0	0	0	0
All	All	8375	0	4194	466	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 38.

The worst 5 of 466 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:92:G:C6	1:A:93:A:N6	2.24	1.06
1:A:282:A:O2'	1:A:283:A:H5'	1.58	1.02
1:A:197:C:N3	1:A:198:U:C5	2.28	1.01
1:A:48:G:N2	1:A:59:U:C5	2.31	0.99
1:A:168:U:H4'	1:A:169:G:OP1	1.64	0.98

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)
1:A:279:C:O2'	1:A:336:G:O2'[3_555]	2.01	0.19

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	389/394 (98%)	191 (49%)	39 (10%)

5 of 191 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	9	G
1	A	10	G
1	A	12	A
1	A	13	U

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	291	G
1	A	356	A
1	A	297	A
1	A	334	U
1	A	374	G

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](#)

Of 16 ligands modelled in this entry, 15 are monoatomic - leaving 1 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	$\# Z > 2$
2	GDE	A	401	3	11,11,12	3.24	7 (63%)	15,15,17	1.73	3 (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	GDE	A	401	3	-	2/2/2/4	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GDE	CAG-CAJ	5.60	1.46	1.38
2	A	401	GDE	CAJ-CAL	-5.05	1.34	1.40
2	A	401	GDE	OAD-CAJ	4.07	1.44	1.36
2	A	401	GDE	CAK-CAH	3.24	1.57	1.47
2	A	401	GDE	CAF-CAI	3.02	1.43	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	GDE	CAF-CAK-CAH	3.73	127.51	119.98
2	A	401	GDE	OAC-CAI-CAF	3.08	127.77	119.45
2	A	401	GDE	OAC-CAI-CAL	-2.66	111.05	117.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GDE	OAB-CAH-CAK-CAF
2	A	401	GDE	OAB-CAH-CAK-CAG

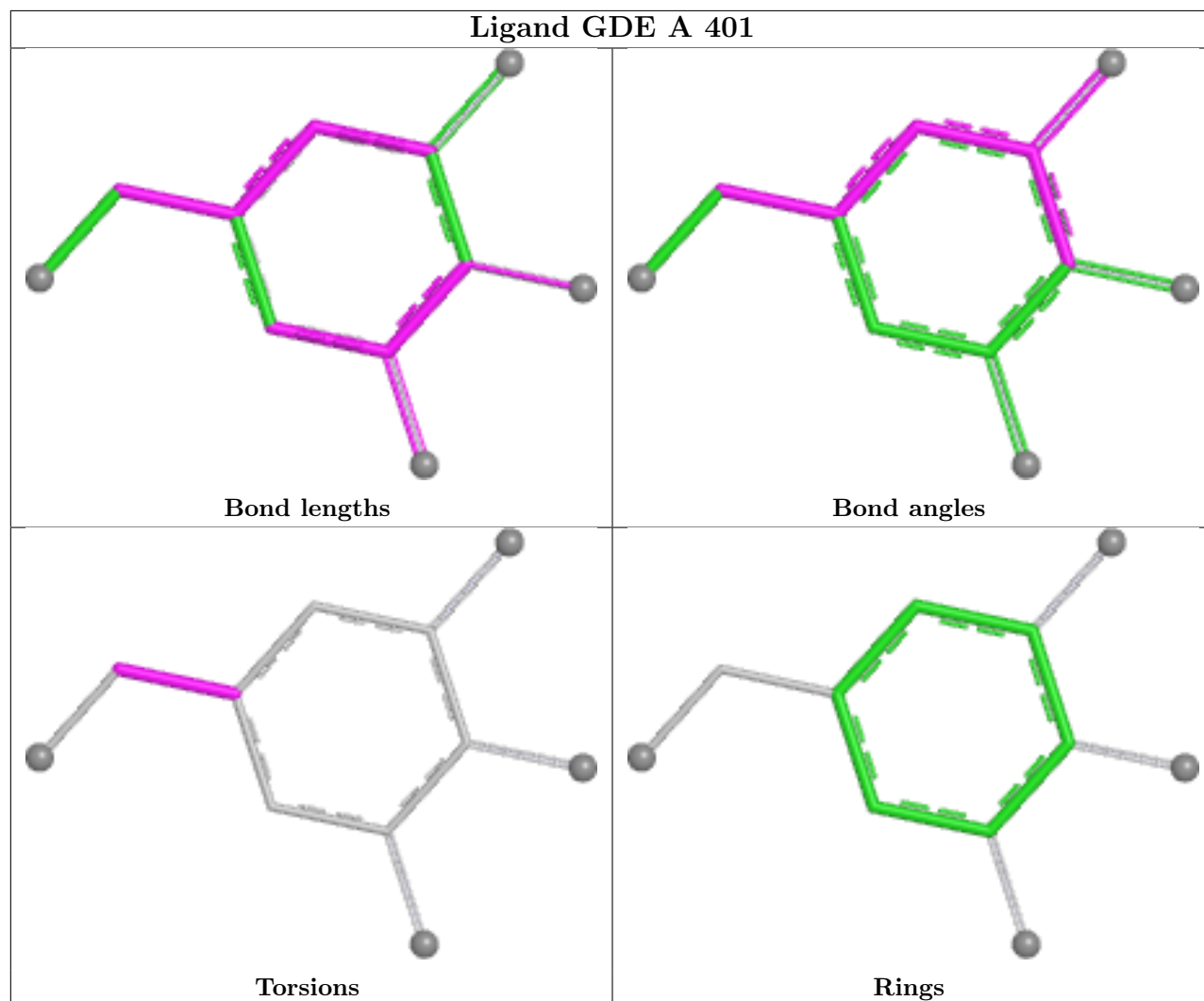
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	GDE	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.



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	390/394 (98%)	0.15	28 (7%) 21 15	134, 215, 350, 427	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	G	24.6
1	A	370	A	8.3
1	A	237	A	7.2
1	A	2	U	5.8
1	A	214	U	5.5

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](#)

There are no oligosaccharides 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, 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	NA	A	412	1/1	-0.28	0.28	264,264,264,264	0
3	MG	A	416	1/1	0.45	0.33	166,166,166,166	0

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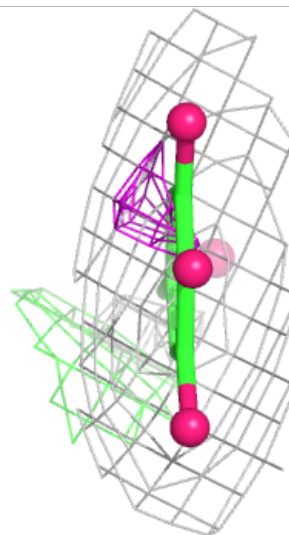
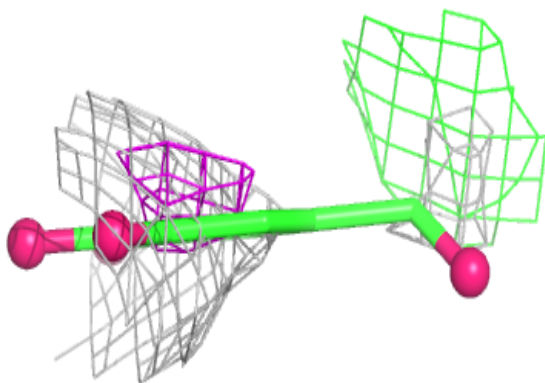
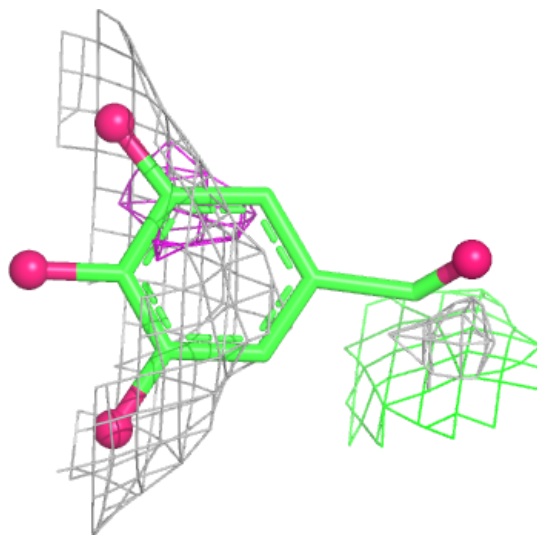
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	405	1/1	0.56	0.30	238,238,238,238	0
4	NA	A	410	1/1	0.68	0.20	162,162,162,162	0
2	GDE	A	401	11/12	0.69	0.16	112,119,146,181	0
3	MG	A	403	1/1	0.74	0.32	180,180,180,180	0
3	MG	A	415	1/1	0.78	0.18	160,160,160,160	0
4	NA	A	409	1/1	0.80	0.15	164,164,164,164	0
3	MG	A	402	1/1	0.82	0.30	155,155,155,155	0
4	NA	A	411	1/1	0.91	0.12	159,159,159,159	0
3	MG	A	406	1/1	0.91	0.08	224,224,224,224	0
3	MG	A	404	1/1	0.93	0.05	187,187,187,187	0
4	NA	A	408	1/1	0.93	0.05	172,172,172,172	0
3	MG	A	413	1/1	0.94	0.14	179,179,179,179	0
3	MG	A	407	1/1	0.97	0.07	186,186,186,186	0
3	MG	A	414	1/1	0.99	0.03	164,164,164,164	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 GDE 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 [i](#)

There are no such residues in this entry.