



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:01 PM UTC

PDB ID : 9FTR / pdb_00009ftr
Title : Drosophila golgi alpha-mannosidase II (dGMII) in complex with amide modified swainsonine-configured alkyl indolizidine
Authors : Bennett, M.; Koemans, T.; Overkleeft, H.S.; Davies, G.J.
Deposited on : 2024-06-25
Resolution : 2.14 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

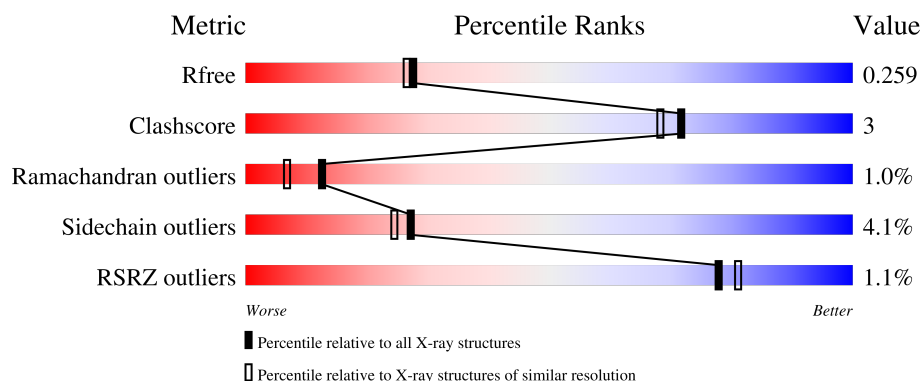
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	1033	77% 17% • •

2 Entry composition [i](#)

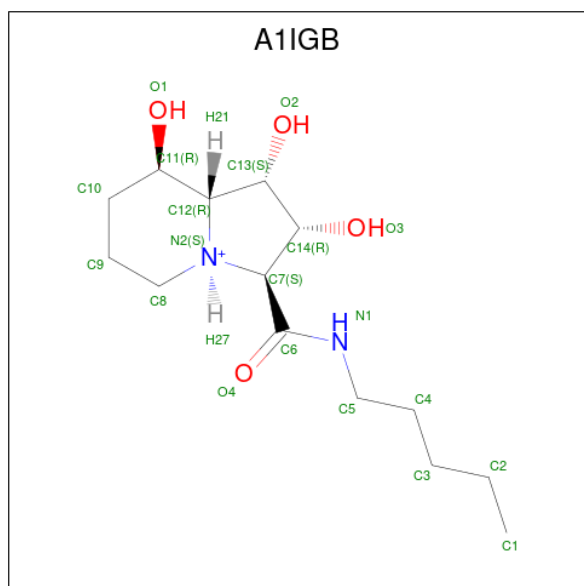
There are 5 unique types of molecules in this entry. The entry contains 8337 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-mannosidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	999	7921	5053	1375	1454	39	0	2	0

- Molecule 2 is amide modified swainsonine-configured alkyl indolizidine (CCD ID: A1IGB) (formula: $C_{14}H_{27}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	18	12	2	4	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0

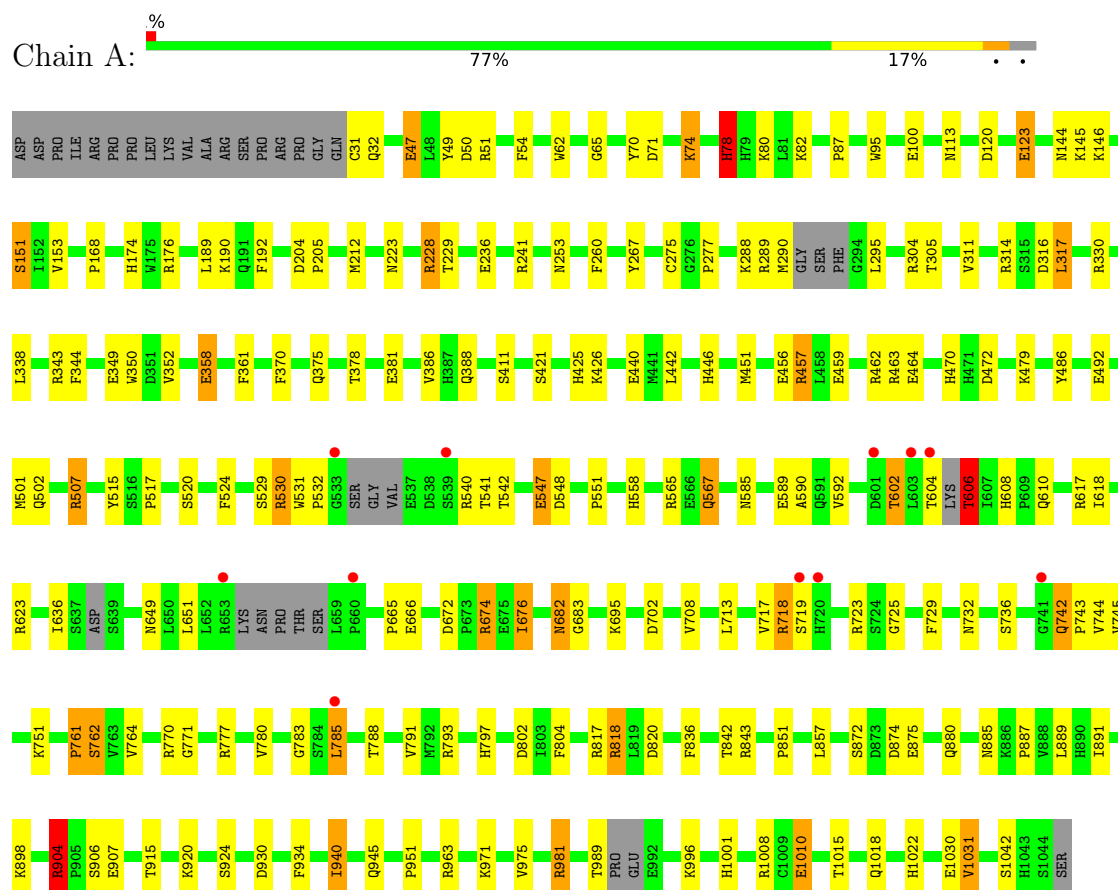
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	309	Total O 309 309	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Alpha-mannosidase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.11Å 91.94Å 133.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.68 – 2.14 57.68 – 2.14	Depositor EDS
% Data completeness (in resolution range)	100.0 (57.68-2.14) 100.0 (57.68-2.14)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.179 , 0.259 0.179 , 0.259	Depositor DCC
R_{free} test set	1969 reflections (2.54%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8337	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, ZN, A1IGB

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	0.97	6/8135 (0.1%)	1.67	128/11064 (1.2%)

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	12

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	HIS	CD2-NE2	-17.15	1.19	1.37
1	A	78	HIS	CG-CD2	10.50	1.47	1.35
1	A	78	HIS	CE1-NE2	10.33	1.42	1.32
1	A	1010	GLU	CD-OE2	9.47	1.43	1.25
1	A	674	ARG	NE-CZ	5.92	1.39	1.33
1	A	520	SER	CA-CB	-5.02	1.45	1.53

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	606	THR	CA-CB-OG1	-14.48	87.88	109.60
1	A	78	HIS	CA-CB-CG	-11.25	102.55	113.80
1	A	585	ASN	CB-CA-C	10.99	129.61	111.26
1	A	541	THR	CA-CB-OG1	-10.35	94.07	109.60
1	A	836	PHE	CA-CB-CG	9.37	123.17	113.80
1	A	1010	GLU	CG-CD-OE2	9.19	139.53	118.40
1	A	277	PRO	N-CA-C	8.95	125.05	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	971	LYS	N-CA-CB	8.75	123.10	110.16
1	A	305	THR	CA-CB-OG1	-8.62	96.66	109.60
1	A	425	HIS	CA-CB-CG	-8.39	105.41	113.80
1	A	446	HIS	CA-CB-CG	-8.32	105.48	113.80
1	A	672	ASP	CB-CA-C	8.22	121.44	109.11
1	A	456	GLU	N-CA-CB	8.05	121.69	110.01
1	A	123	GLU	CB-CG-CD	7.99	126.19	112.60
1	A	742	GLN	CB-CA-C	7.93	123.50	110.97
1	A	751	LYS	CA-CB-CG	7.71	129.53	114.10
1	A	1010	GLU	CG-CD-OE1	-7.69	100.71	118.40
1	A	358	GLU	CB-CG-CD	7.65	125.61	112.60
1	A	253	ASN	CA-C-N	7.50	130.64	120.44
1	A	253	ASN	C-N-CA	7.50	130.64	120.44
1	A	904	ARG	CB-CA-C	-7.49	98.08	108.86
1	A	788	THR	CA-CB-OG1	-7.40	98.50	109.60
1	A	934	PHE	CB-CA-C	7.34	121.34	109.90
1	A	236	GLU	CB-CG-CD	7.21	124.85	112.60
1	A	78	HIS	CB-CG-ND1	-7.20	111.91	122.70
1	A	421	SER	CA-C-N	7.19	130.59	122.83
1	A	421	SER	C-N-CA	7.19	130.59	122.83
1	A	51	ARG	CB-CG-CD	-7.11	94.94	111.30
1	A	451	MET	CG-SD-CE	7.04	116.38	100.90
1	A	501	MET	CG-SD-CE	-6.82	85.90	100.90
1	A	729	PHE	CA-CB-CG	6.79	120.59	113.80
1	A	1030	GLU	N-CA-CB	6.79	120.08	109.83
1	A	456	GLU	CB-CG-CD	6.71	124.01	112.60
1	A	547	GLU	N-CA-CB	6.59	121.53	110.32
1	A	370	PHE	N-CA-CB	6.57	119.88	110.16
1	A	78	HIS	ND1-CG-CD2	6.47	112.57	106.10
1	A	502	GLN	CB-CA-C	6.46	121.50	110.79
1	A	793	ARG	CD-NE-CZ	6.37	133.32	124.40
1	A	520	SER	CA-CB-OG	-6.37	98.36	111.10
1	A	47	GLU	CB-CG-CD	-6.37	101.78	112.60
1	A	745	VAL	CA-C-N	6.36	130.88	122.30
1	A	745	VAL	C-N-CA	6.36	130.88	122.30
1	A	817	ARG	NE-CZ-NH1	6.36	127.86	121.50
1	A	31	CYS	CB-CA-C	-6.32	98.09	110.10
1	A	920	LYS	N-CA-CB	6.32	119.51	110.16
1	A	457	ARG	CB-CG-CD	-6.23	96.98	111.30
1	A	168	PRO	N-CA-CB	-6.20	96.87	103.38
1	A	1015	THR	CA-CB-OG1	-6.20	100.31	109.60
1	A	602	THR	CA-CB-OG1	-6.18	100.34	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	608	HIS	CB-CA-C	6.15	118.41	108.87
1	A	818	ARG	NE-CZ-NH2	-6.15	113.67	119.20
1	A	78	HIS	CG-ND1-CE1	-6.15	98.85	109.30
1	A	151	SER	CA-CB-OG	-6.13	98.85	111.10
1	A	80	LYS	CB-CG-CD	6.12	125.38	111.30
1	A	50	ASP	CB-CA-C	6.05	122.29	110.67
1	A	875	GLU	CB-CA-C	6.05	120.32	111.73
1	A	542	THR	CA-CB-OG1	-6.00	100.60	109.60
1	A	718	ARG	CB-CA-C	6.00	119.67	109.53
1	A	459	GLU	N-CA-CB	5.99	118.76	110.07
1	A	842	THR	CA-CB-OG1	-5.99	100.61	109.60
1	A	682	ASN	CB-CA-C	-5.96	99.76	110.37
1	A	817	ARG	CD-NE-CZ	5.93	132.71	124.40
1	A	904	ARG	N-CA-CB	5.93	117.21	110.03
1	A	316	ASP	CA-C-N	5.92	128.13	120.44
1	A	316	ASP	C-N-CA	5.92	128.13	120.44
1	A	381	GLU	N-CA-CB	5.90	118.57	110.01
1	A	797	HIS	CB-CA-C	5.88	120.50	110.56
1	A	51	ARG	CG-CD-NE	-5.86	99.11	112.00
1	A	145	LYS	CB-CG-CD	5.83	124.70	111.30
1	A	1001	HIS	CA-CB-CG	-5.80	108.00	113.80
1	A	153	VAL	N-CA-C	-5.78	104.70	111.00
1	A	975	VAL	CA-C-N	-5.78	117.20	122.80
1	A	975	VAL	C-N-CA	-5.78	117.20	122.80
1	A	386	VAL	N-CA-CB	5.75	117.28	110.55
1	A	49	TYR	N-CA-CB	5.71	119.02	110.22
1	A	288	LYS	CG-CD-CE	5.68	124.37	111.30
1	A	524	PHE	CA-CB-CG	5.66	119.46	113.80
1	A	289	ARG	N-CA-CB	-5.66	101.00	110.22
1	A	459	GLU	CB-CG-CD	-5.65	102.99	112.60
1	A	463	ARG	CA-CB-CG	-5.62	102.85	114.10
1	A	479	LYS	CB-CG-CD	5.61	124.21	111.30
1	A	113	ASN	CA-CB-CG	-5.61	106.99	112.60
1	A	361	PHE	CA-CB-CG	5.58	119.38	113.80
1	A	229	THR	CA-CB-OG1	-5.56	101.26	109.60
1	A	649	ASN	CB-CA-C	5.56	119.77	109.70
1	A	804	PHE	CA-CB-CG	5.55	119.35	113.80
1	A	317	LEU	N-CA-CB	-5.51	102.01	110.01
1	A	78	HIS	CG-CD2-NE2	-5.51	101.69	107.20
1	A	507	ARG	CA-CB-CG	-5.48	103.14	114.10
1	A	146	LYS	N-CA-CB	5.47	118.09	109.94
1	A	761	PRO	N-CA-C	-5.47	101.91	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	ARG	CA-CB-CG	-5.46	103.17	114.10
1	A	567	GLN	CB-CA-C	5.45	120.47	109.68
1	A	820	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	311	VAL	N-CA-CB	5.45	117.94	110.54
1	A	486	TYR	N-CA-CB	5.43	118.11	110.12
1	A	702	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	817	ARG	NE-CZ-NH2	-5.37	114.37	119.20
1	A	463	ARG	N-CA-CB	5.36	117.84	110.07
1	A	666	GLU	CB-CA-C	5.36	119.17	110.22
1	A	378	THR	CA-CB-OG1	-5.34	101.58	109.60
1	A	212	MET	CG-SD-CE	-5.34	89.14	100.90
1	A	530	ARG	CB-CG-CD	-5.33	99.03	111.30
1	A	802	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	189	LEU	N-CA-CB	5.30	117.75	110.07
1	A	695	LYS	CB-CA-C	5.29	120.94	110.42
1	A	770	ARG	CA-C-N	-5.28	117.17	123.08
1	A	770	ARG	C-N-CA	-5.28	117.17	123.08
1	A	100	GLU	CB-CA-C	5.28	119.55	110.79
1	A	530	ARG	CG-CD-NE	-5.28	100.39	112.00
1	A	723	ARG	CB-CA-C	5.27	118.45	109.80
1	A	192	PHE	CB-CA-C	5.26	118.44	109.24
1	A	267	TYR	N-CA-CB	-5.25	102.15	110.28
1	A	915	THR	CA-CB-OG1	-5.20	101.80	109.60
1	A	456	GLU	CB-CA-C	-5.20	102.72	110.88
1	A	718	ARG	CA-CB-CG	-5.16	103.78	114.10
1	A	120	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	981	ARG	CD-NE-CZ	5.13	131.59	124.40
1	A	751	LYS	CB-CG-CD	-5.09	99.58	111.30
1	A	934	PHE	CA-CB-CG	-5.08	108.72	113.80
1	A	996	LYS	CB-CA-C	-5.08	102.22	109.84
1	A	32	GLN	CB-CA-C	-5.06	100.56	109.62
1	A	314	ARG	CB-CA-C	5.06	119.45	110.85
1	A	665	PRO	N-CA-C	5.04	122.84	112.47
1	A	889	LEU	CA-C-N	5.04	128.62	121.42
1	A	889	LEU	C-N-CA	5.04	128.62	121.42
1	A	290	MET	CB-CA-C	-5.03	100.55	110.10
1	A	228	ARG	N-CA-CB	5.01	117.33	110.57

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	304	ARG	Sidechain
1	A	330	ARG	Sidechain
1	A	457	ARG	Sidechain
1	A	507	ARG	Sidechain
1	A	547	GLU	Peptide
1	A	548	ASP	Peptide
1	A	602	THR	Peptide
1	A	623	ARG	Sidechain
1	A	78	HIS	Sidechain
1	A	843	ARG	Sidechain
1	A	904	ARG	Sidechain
1	A	963	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	7921	0	7545	51	4
2	A	18	0	0	1	0
3	A	88	0	132	8	0
4	A	1	0	0	0	0
5	A	309	0	0	7	0
All	All	8337	0	7677	52	4

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 (52) 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:717:VAL:O	1:A:732:ASN:ND2	2.16	0.79
1:A:989:THR:HG22	5:A:1264:HOH:O	1.86	0.75
1:A:761:PRO:O	1:A:762:SER:HB2	1.92	0.68
1:A:940:ILE:HD12	1:A:940:ILE:H	1.58	0.66
1:A:82:LYS:CD	5:A:1476:HOH:O	2.43	0.66
1:A:604:THR:OG1	1:A:606:THR:HB	2.02	0.60
1:A:241:ARG:HH21	3:A:1122:EDO:H11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:951:PRO:HG3	3:A:1120:EDO:H21	1.84	0.58
1:A:241:ARG:HH21	3:A:1122:EDO:C1	2.17	0.57
1:A:725:GLY:HA3	1:A:874:ASP:CG	2.32	0.55
1:A:1018:GLN:CG	5:A:1507:HOH:O	2.54	0.55
1:A:904:ARG:HB2	5:A:1406:HOH:O	2.06	0.55
1:A:70:TYR:H	3:A:1117:EDO:H11	1.72	0.54
1:A:590:ALA:HB1	1:A:618:ILE:HD11	1.90	0.54
1:A:54:PHE:HB3	3:A:1114:EDO:H11	1.93	0.50
1:A:426:LYS:HD3	1:A:851:PRO:O	2.13	0.49
1:A:717:VAL:HG12	1:A:718:ARG:H	1.78	0.49
1:A:71:ASP:O	1:A:74:LYS:HB2	2.13	0.49
1:A:54:PHE:CB	3:A:1114:EDO:H11	2.43	0.48
1:A:205:PRO:O	1:A:228:ARG:HB2	2.13	0.48
1:A:470:HIS:CD2	1:A:472:ASP:H	2.32	0.47
1:A:223:ASN:HD22	1:A:260:PHE:HD2	1.61	0.47
1:A:344:PHE:H	1:A:349:GLU:CD	2.22	0.47
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.50	0.47
1:A:123:GLU:OE2	1:A:358:GLU:OE2	2.34	0.46
1:A:515:TYR:CZ	1:A:517:PRO:HG3	2.50	0.46
1:A:464:GLU:HA	1:A:464:GLU:OE1	2.16	0.46
1:A:683:GLY:HA3	1:A:771:GLY:O	2.15	0.45
1:A:777:ARG:HG2	1:A:891:ILE:HG22	1.97	0.45
1:A:717:VAL:HG12	1:A:718:ARG:N	2.32	0.45
1:A:592:VAL:HA	1:A:617:ARG:O	2.17	0.44
1:A:87:PRO:HA	1:A:338:LEU:O	2.18	0.44
1:A:558:HIS:HB3	1:A:930:ASP:HB2	1.99	0.44
1:A:440:GLU:OE2	1:A:462:ARG:HD3	2.18	0.44
1:A:295:LEU:HD23	5:A:1454:HOH:O	2.18	0.43
1:A:764:VAL:HB	3:A:1112:EDO:H11	1.99	0.43
1:A:551:PRO:O	1:A:636:ILE:HG22	2.18	0.43
1:A:818:ARG:HD3	1:A:857:LEU:HA	2.00	0.43
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.84	0.43
1:A:62:TRP:CD2	1:A:65:GLY:HA3	2.54	0.43
1:A:676:ILE:HD13	1:A:676:ILE:HA	1.88	0.43
1:A:780:VAL:O	1:A:887:PRO:HA	2.19	0.43
1:A:945:GLN:HG2	5:A:1323:HOH:O	2.19	0.43
1:A:651:LEU:HD11	1:A:744:VAL:CG1	2.49	0.42
1:A:981:ARG:HD3	1:A:1031:VAL:O	2.20	0.42
1:A:531:TRP:HA	1:A:532:PRO:HA	1.73	0.41
1:A:344:PHE:HB3	1:A:350:TRP:CE2	2.55	0.41
1:A:713:LEU:HB2	1:A:791:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:PRO:HD2	5:A:1354:HOH:O	2.20	0.41
1:A:940:ILE:H	1:A:940:ILE:CD1	2.22	0.41
2:A:1101:A1IGB:N1	3:A:1111:EDO:H21	2.36	0.41
1:A:1008:ARG:HB3	1:A:1042:SER:HB2	2.03	0.40

All (4) 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:78:HIS:NE2	1:A:1010:GLU:OE2[4_445]	1.30	0.90
1:A:78:HIS:NE2	1:A:1022:HIS:ND1[4_445]	1.71	0.49
1:A:78:HIS:CD2	1:A:1010:GLU:OE2[4_445]	1.99	0.21
1:A:78:HIS:CD2	1:A:1022:HIS:ND1[4_445]	2.17	0.03

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	987/1033 (96%)	945 (96%)	32 (3%)	10 (1%)	12 7

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	719	SER
1	A	411	SER
1	A	785	LEU
1	A	540	ARG
1	A	783	GLY
1	A	95	TRP
1	A	907	GLU
1	A	762	SER
1	A	708	VAL

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Mol	Chain	Res	Type
1	A	204	ASP

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	839/918 (91%)	805 (96%)	34 (4%)	27	24

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLU
1	A	74	LYS
1	A	78	HIS
1	A	144	ASN
1	A	151	SER
1	A	190	LYS
1	A	275	CYS
1	A	317	LEU
1	A	352	VAL
1	A	375	GLN
1	A	388	GLN
1	A	492	GLU
1	A	529	SER
1	A	530	ARG
1	A	565	ARG
1	A	567	GLN
1	A	589	GLU
1	A	606	THR
1	A	610	GLN
1	A	674	ARG
1	A	676	ILE
1	A	682	ASN
1	A	736	SER
1	A	742	GLN
1	A	785	LEU

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Mol	Chain	Res	Type
1	A	872	SER
1	A	880	GLN
1	A	885	ASN
1	A	898	LYS
1	A	904	ARG
1	A	906	SER
1	A	924	SER
1	A	940	ILE
1	A	1031	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	117	HIS
1	A	119	HIS
1	A	223	ASN
1	A	249	GLN
1	A	253	ASN
1	A	371	ASN
1	A	608	HIS
1	A	698	GLN
1	A	709	HIS
1	A	778	ASN
1	A	812	GLN
1	A	866	GLN
1	A	923	GLN
1	A	1019	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 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
3	EDO	A	1106	-	3,3,3	0.37	0	2,2,2	0.30	0
3	EDO	A	1111	-	3,3,3	0.50	0	2,2,2	0.54	0
3	EDO	A	1103	-	3,3,3	0.14	0	2,2,2	0.16	0
3	EDO	A	1117	-	3,3,3	0.29	0	2,2,2	0.83	0
3	EDO	A	1113	-	3,3,3	0.17	0	2,2,2	0.40	0
3	EDO	A	1104	-	3,3,3	0.09	0	2,2,2	0.97	0
2	A1IGB	A	1101	4	19,19,21	1.43	2 (10%)	21,27,29	1.82	6 (28%)
3	EDO	A	1119	-	3,3,3	0.31	0	2,2,2	0.21	0
3	EDO	A	1118	-	3,3,3	0.25	0	2,2,2	0.66	0
3	EDO	A	1123	-	3,3,3	0.11	0	2,2,2	0.12	0
3	EDO	A	1120	-	3,3,3	0.18	0	2,2,2	0.28	0
3	EDO	A	1121	-	3,3,3	0.17	0	2,2,2	0.14	0
3	EDO	A	1114	-	3,3,3	0.26	0	2,2,2	0.73	0
3	EDO	A	1102	-	3,3,3	0.16	0	2,2,2	0.73	0
3	EDO	A	1116	-	3,3,3	0.29	0	2,2,2	0.38	0
3	EDO	A	1109	-	3,3,3	0.32	0	2,2,2	0.10	0
3	EDO	A	1107	-	3,3,3	0.46	0	2,2,2	0.70	0
3	EDO	A	1112	-	3,3,3	0.27	0	2,2,2	0.39	0
3	EDO	A	1122	-	3,3,3	0.17	0	2,2,2	0.63	0
3	EDO	A	1108	-	3,3,3	0.20	0	2,2,2	1.17	0
3	EDO	A	1105	-	3,3,3	0.39	0	2,2,2	0.11	0
3	EDO	A	1115	-	3,3,3	0.45	0	2,2,2	0.71	0
3	EDO	A	1110	-	3,3,3	0.20	0	2,2,2	0.57	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
3	EDO	A	1106	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	1111	-	-	0/1/1/1	-
3	EDO	A	1103	-	-	0/1/1/1	-
3	EDO	A	1117	-	-	1/1/1/1	-
3	EDO	A	1113	-	-	0/1/1/1	-
3	EDO	A	1104	-	-	0/1/1/1	-
2	A1IGB	A	1101	4	-	4/8/38/40	0/2/2/2
3	EDO	A	1119	-	-	1/1/1/1	-
3	EDO	A	1118	-	-	1/1/1/1	-
3	EDO	A	1123	-	-	1/1/1/1	-
3	EDO	A	1120	-	-	0/1/1/1	-
3	EDO	A	1121	-	-	1/1/1/1	-
3	EDO	A	1114	-	-	1/1/1/1	-
3	EDO	A	1102	-	-	0/1/1/1	-
3	EDO	A	1116	-	-	1/1/1/1	-
3	EDO	A	1109	-	-	1/1/1/1	-
3	EDO	A	1107	-	-	0/1/1/1	-
3	EDO	A	1112	-	-	1/1/1/1	-
3	EDO	A	1122	-	-	1/1/1/1	-
3	EDO	A	1108	-	-	0/1/1/1	-
3	EDO	A	1105	-	-	1/1/1/1	-
3	EDO	A	1115	-	-	1/1/1/1	-
3	EDO	A	1110	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	A1IGB	C7-N2	5.14	1.53	1.47
2	A	1101	A1IGB	C8-N2	2.36	1.51	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	A1IGB	C14-C7-C6	3.86	117.87	110.30
2	A	1101	A1IGB	C8-N2-C12	3.62	116.24	112.05
2	A	1101	A1IGB	O1-C11-C10	-2.98	102.69	109.99
2	A	1101	A1IGB	C9-C8-N2	2.64	116.48	110.46
2	A	1101	A1IGB	C7-C6-N1	2.31	120.25	116.05
2	A	1101	A1IGB	C10-C9-C8	-2.22	107.83	110.75

There are no chirality outliers.

All (18) torsion outliers are listed below:

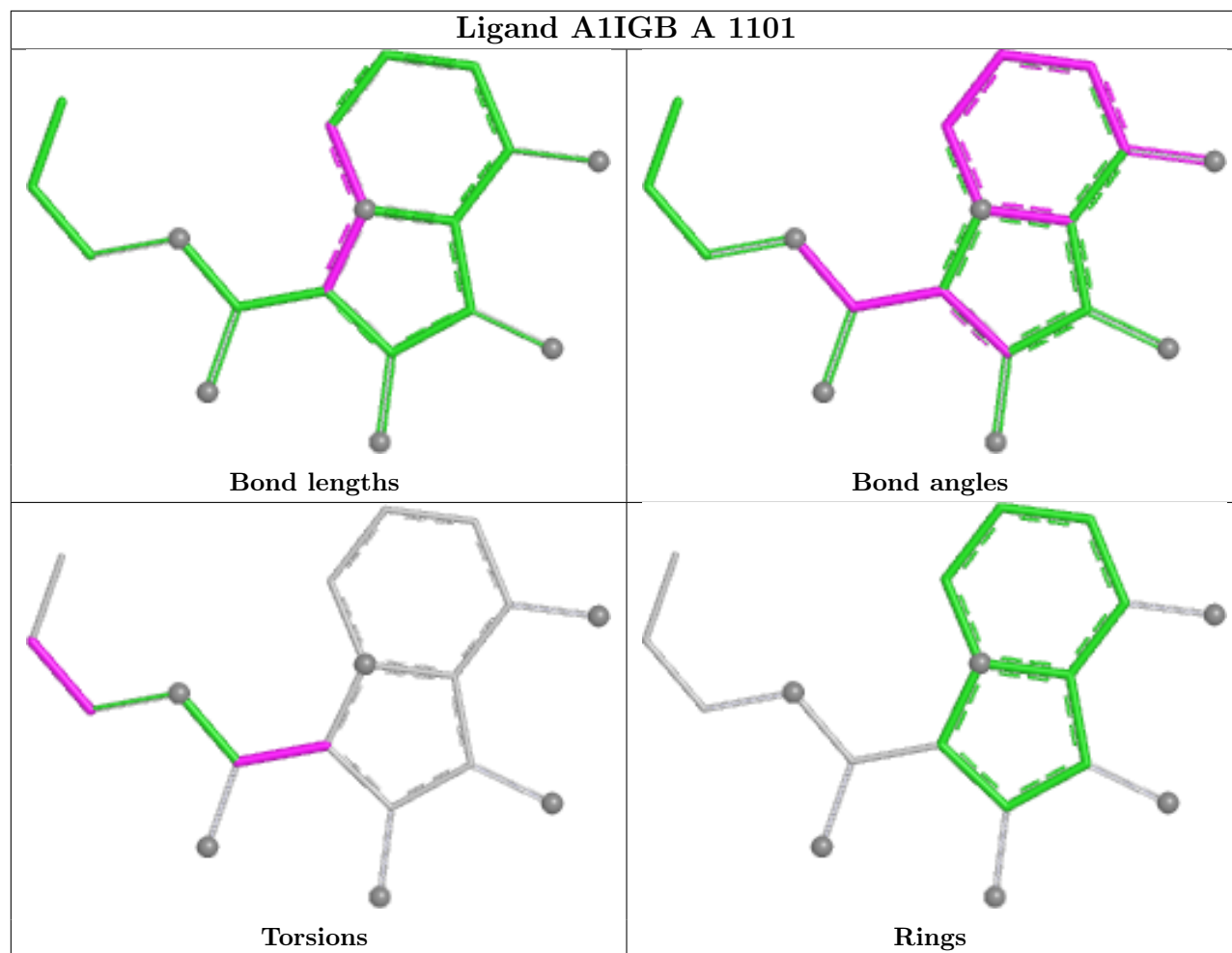
Mol	Chain	Res	Type	Atoms
3	A	1109	EDO	O1-C1-C2-O2
3	A	1115	EDO	O1-C1-C2-O2
2	A	1101	A1IGB	O4-C6-C7-C14
2	A	1101	A1IGB	O4-C6-C7-N2
2	A	1101	A1IGB	C3-C4-C5-N1
3	A	1122	EDO	O1-C1-C2-O2
3	A	1114	EDO	O1-C1-C2-O2
3	A	1117	EDO	O1-C1-C2-O2
3	A	1110	EDO	O1-C1-C2-O2
3	A	1119	EDO	O1-C1-C2-O2
3	A	1121	EDO	O1-C1-C2-O2
3	A	1123	EDO	O1-C1-C2-O2
2	A	1101	A1IGB	N1-C6-C7-N2
3	A	1116	EDO	O1-C1-C2-O2
3	A	1105	EDO	O1-C1-C2-O2
3	A	1106	EDO	O1-C1-C2-O2
3	A	1112	EDO	O1-C1-C2-O2
3	A	1118	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1111	EDO	1	0
3	A	1117	EDO	1	0
2	A	1101	A1IGB	1	0
3	A	1120	EDO	1	0
3	A	1114	EDO	2	0
3	A	1112	EDO	1	0
3	A	1122	EDO	2	0

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



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	999/1033 (96%)	-0.44	11 (1%) 78 81	15, 35, 60, 102	2 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	720	HIS	2.7
1	A	533	GLY	2.6
1	A	604	THR	2.4
1	A	653	ARG	2.3
1	A	785	LEU	2.3
1	A	539	SER	2.2
1	A	601	ASP	2.2
1	A	719	SER	2.1
1	A	603	LEU	2.0
1	A	741	GLY	2.0
1	A	660	PRO	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](#)

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,

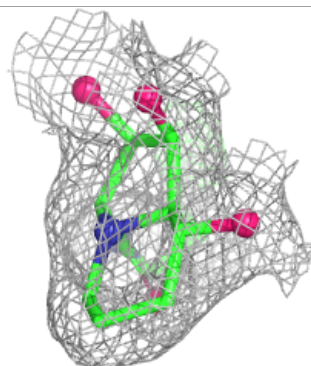
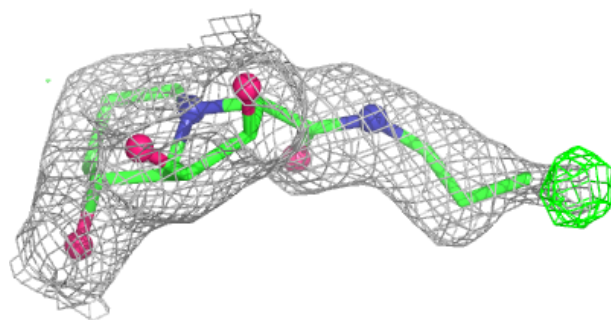
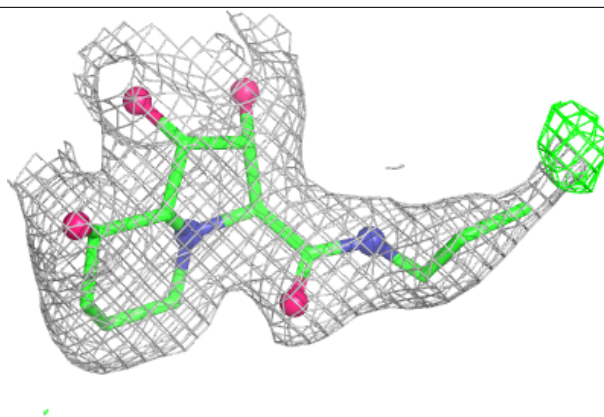
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	1109	4/4	0.78	0.17	55,55,61,74	0
3	EDO	A	1119	4/4	0.80	0.17	59,60,67,70	0
3	EDO	A	1118	4/4	0.88	0.15	54,61,62,69	0
3	EDO	A	1117	4/4	0.88	0.12	49,60,62,69	0
3	EDO	A	1123	4/4	0.90	0.09	50,51,55,64	0
3	EDO	A	1114	4/4	0.91	0.09	53,62,64,69	0
3	EDO	A	1110	4/4	0.92	0.10	48,56,58,61	0
3	EDO	A	1122	4/4	0.92	0.09	40,51,52,57	0
3	EDO	A	1116	4/4	0.92	0.10	54,54,61,63	0
3	EDO	A	1113	4/4	0.93	0.08	48,50,51,68	0
3	EDO	A	1115	4/4	0.93	0.13	41,55,59,78	0
3	EDO	A	1111	4/4	0.94	0.10	47,48,50,52	0
3	EDO	A	1108	4/4	0.94	0.10	37,38,45,47	0
3	EDO	A	1107	4/4	0.95	0.08	40,43,49,59	0
3	EDO	A	1105	4/4	0.95	0.07	35,41,42,54	0
3	EDO	A	1120	4/4	0.95	0.07	40,49,50,61	0
3	EDO	A	1112	4/4	0.95	0.12	48,48,49,56	0
3	EDO	A	1106	4/4	0.95	0.09	44,47,48,50	0
2	A1IGB	A	1101	18/20	0.96	0.06	18,23,41,44	0
3	EDO	A	1103	4/4	0.96	0.07	33,33,40,44	0
3	EDO	A	1104	4/4	0.97	0.07	38,38,38,41	0
3	EDO	A	1121	4/4	0.97	0.06	42,46,46,53	0
3	EDO	A	1102	4/4	0.98	0.05	19,26,28,32	0
4	ZN	A	1124	1/1	1.00	0.02	27,27,27,27	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 A1IGB A 1101:

$2mF_o-DF_c$ (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.