



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:13 PM UTC

PDB ID : 9FTQ / pdb_00009ftq
Title : Drosophila golgi alpha-mannosidase II (dGMII) in complex with swainsonine
-configured alkyl indolizidine
Authors : Bennett, M.; Koemans, T.; Overkleeft, H.S.; Davies, G.J.
Deposited on : 2024-06-25
Resolution : 2.47 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

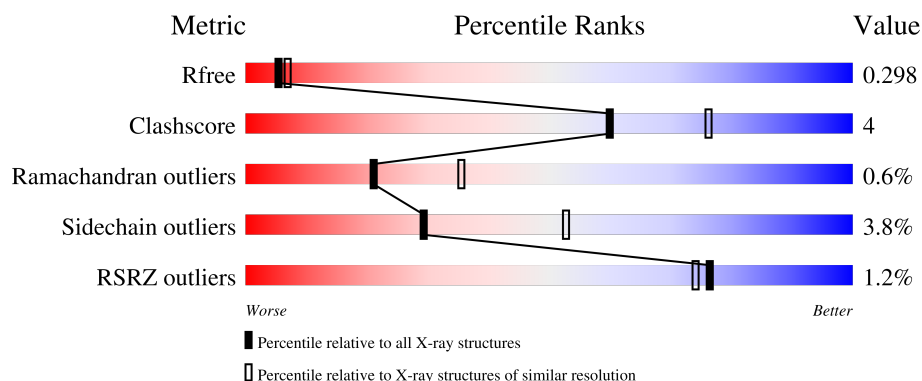
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

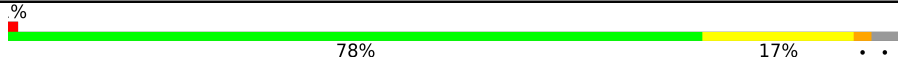
The reported resolution of this entry is 2.47 Å.

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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	

2 Entry composition [i](#)

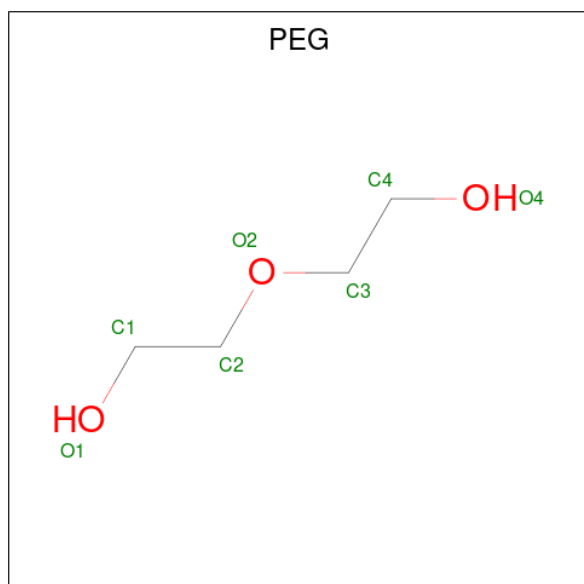
There are 5 unique types of molecules in this entry. The entry contains 8082 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

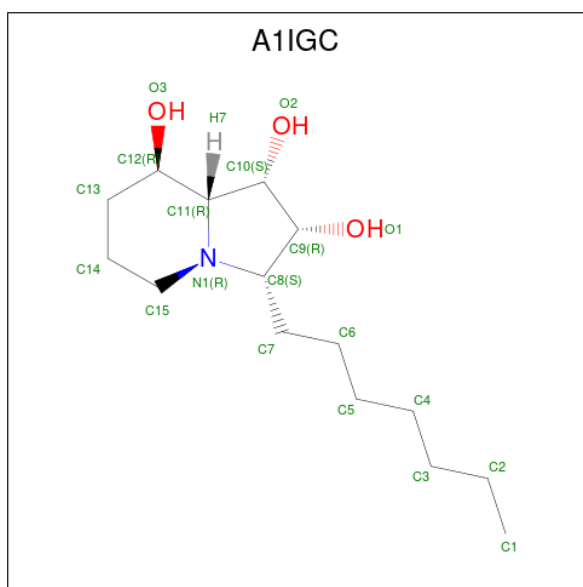
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1006	Total	C	N	O	S	0	0	0
			7970	5084	1378	1469	39			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is swainsonine-configured alkyl indolizidine (CCD ID: A1IGC) (formula: $C_{15}H_{29}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	8	1	3		

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

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

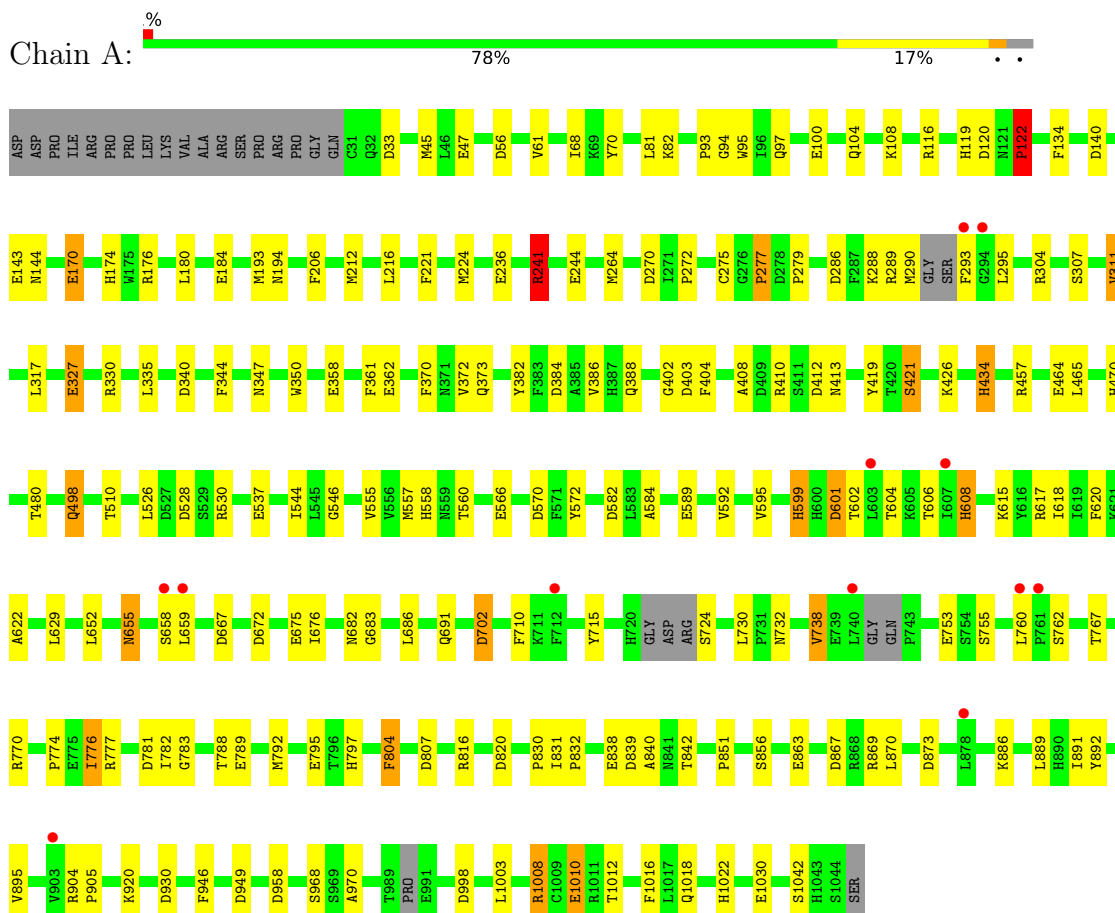
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	85	Total	O	0	0
			85	85		

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	88.91Å 90.91Å 132.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.98 – 2.47 74.98 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.9 (74.98-2.47) 99.9 (74.98-2.47)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.208 , 0.298 0.208 , 0.298	Depositor DCC
R_{free} test set	1055 reflections (2.69%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8082	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: ZN, A1IGC, PEG

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	0.62	0/8186	1.54	90/11140 (0.8%)

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	4

There are no bond length outliers.

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1010	GLU	CB-CG-CD	10.02	129.64	112.60
1	A	599	HIS	CA-CB-CG	9.82	123.62	113.80
1	A	797	HIS	CB-CA-C	9.40	122.78	111.22
1	A	498	GLN	CB-CA-C	-9.23	96.04	110.81
1	A	608	HIS	CA-CB-CG	8.84	122.64	113.80
1	A	1010	GLU	CB-CA-C	8.41	123.90	109.51
1	A	608	HIS	CB-CA-C	7.57	119.20	108.68
1	A	464	GLU	CB-CG-CD	7.36	125.11	112.60
1	A	311	VAL	N-CA-CB	7.32	118.63	110.51
1	A	1008	ARG	CD-NE-CZ	7.21	134.49	124.40
1	A	1010	GLU	CG-CD-OE2	7.19	134.94	118.40
1	A	361	PHE	CA-CB-CG	6.88	120.67	113.80
1	A	386	VAL	N-CA-CB	6.86	118.58	110.55
1	A	434	HIS	CA-CB-CG	-6.83	106.97	113.80
1	A	120	ASP	CA-CB-CG	6.80	119.40	112.60
1	A	702	ASP	CA-CB-CG	6.72	119.32	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	691	GLN	CB-CA-C	6.61	121.48	111.18
1	A	304	ARG	CB-CA-C	6.56	121.13	109.65
1	A	277	PRO	N-CA-C	6.55	122.36	113.84
1	A	412	ASP	CB-CA-C	6.52	122.32	111.23
1	A	194	ASN	CB-CA-C	6.47	121.74	111.51
1	A	738	VAL	N-CA-CB	6.44	117.74	110.72
1	A	797	HIS	CA-CB-CG	6.38	120.18	113.80
1	A	384	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	293	PHE	CA-CB-CG	6.30	120.10	113.80
1	A	184	GLU	CA-C-N	6.27	126.90	119.94
1	A	184	GLU	C-N-CA	6.27	126.90	119.94
1	A	370	PHE	CA-CB-CG	6.26	120.06	113.80
1	A	710	PHE	CA-CB-CG	6.18	119.98	113.80
1	A	412	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	108	LYS	N-CA-CB	6.11	119.10	110.12
1	A	886	LYS	CB-CA-C	5.99	118.25	109.08
1	A	143	GLU	N-CA-CB	5.96	120.56	110.49
1	A	330	ARG	CD-NE-CZ	5.95	132.73	124.40
1	A	1008	ARG	CA-CB-CG	5.94	125.99	114.10
1	A	270	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	56	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	839	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	170	GLU	CB-CG-CD	5.85	122.54	112.60
1	A	288	LYS	CB-CG-CD	5.77	124.58	111.30
1	A	732	ASN	CB-CA-C	5.76	121.35	111.68
1	A	47	GLU	CB-CG-CD	5.70	122.29	112.60
1	A	388	GLN	CB-CA-C	5.67	120.20	110.79
1	A	620	PHE	CA-CB-CG	5.57	119.37	113.80
1	A	873	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	286	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	820	ASP	CA-C-N	5.50	127.59	120.44
1	A	820	ASP	C-N-CA	5.50	127.59	120.44
1	A	510	THR	CA-CB-OG1	-5.47	101.39	109.60
1	A	602	THR	CA-C-N	5.47	129.03	120.82
1	A	602	THR	C-N-CA	5.47	129.03	120.82
1	A	241	ARG	CA-CB-CG	5.47	125.03	114.10
1	A	958	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	421	SER	CA-C-N	5.46	128.73	122.83
1	A	421	SER	C-N-CA	5.46	128.73	122.83
1	A	544	ILE	CB-CA-C	5.42	118.73	111.19
1	A	546	GLY	CA-C-N	5.40	127.78	120.38
1	A	546	GLY	C-N-CA	5.40	127.78	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	MET	CG-SD-CE	5.39	112.76	100.90
1	A	122	PRO	N-CA-C	5.38	123.55	112.47
1	A	528	ASP	CB-CA-C	5.36	118.71	110.62
1	A	480	THR	CA-CB-OG1	-5.33	101.61	109.60
1	A	905	PRO	CA-C-N	5.32	128.64	120.82
1	A	905	PRO	C-N-CA	5.32	128.64	120.82
1	A	457	ARG	CB-CG-CD	5.30	123.49	111.30
1	A	655	ASN	CB-CA-C	5.29	120.58	110.17
1	A	804	PHE	CA-CB-CG	5.27	119.07	113.80
1	A	920	LYS	N-CA-CB	5.26	117.86	110.12
1	A	795	GLU	CB-CG-CD	5.25	121.53	112.60
1	A	340	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	949	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	601	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	667	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	279	PRO	CA-C-N	5.17	127.21	120.28
1	A	279	PRO	C-N-CA	5.17	127.21	120.28
1	A	404	PHE	CB-CA-C	5.17	120.70	110.42
1	A	56	ASP	CB-CA-C	5.16	120.30	112.00
1	A	1016	PHE	CA-CB-CG	5.15	118.95	113.80
1	A	672	ASP	CB-CA-C	5.14	116.82	109.11
1	A	140	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	457	ARG	CB-CA-C	5.11	120.06	110.70
1	A	781	ASP	CA-C-N	5.11	127.10	120.56
1	A	781	ASP	C-N-CA	5.11	127.10	120.56
1	A	224	MET	CG-SD-CE	5.08	112.09	100.90
1	A	1003	LEU	CB-CA-C	5.07	116.50	108.84
1	A	293	PHE	CB-CA-C	5.06	119.71	110.10
1	A	1030	GLU	CB-CG-CD	5.04	121.16	112.60
1	A	867	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	1012	THR	CA-CB-OG1	-5.02	102.07	109.60
1	A	1008	ARG	NE-CZ-NH1	5.01	126.51	121.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	ARG	Sidechain
1	A	289	ARG	Sidechain
1	A	683	GLY	Peptide
1	A	782	ILE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7970	0	7604	67	0
2	A	14	0	20	2	0
3	A	12	0	0	0	0
4	A	1	0	0	0	0
5	A	85	0	0	1	0
All	All	8082	0	7624	67	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 4.

All (67) 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:1010:GLU:OE2	1:A:1022:HIS:ND1	2.18	0.76
1:A:119:HIS:HE1	5:A:1260:HOH:O	1.69	0.75
1:A:724:SER:HB2	1:A:730:LEU:HB2	1.70	0.74
1:A:617:ARG:HD2	2:A:1102:PEG:H22	1.69	0.73
1:A:1008:ARG:NH1	1:A:1010:GLU:OE2	2.32	0.62
1:A:1010:GLU:CD	1:A:1022:HIS:ND1	2.60	0.60
1:A:81:LEU:HB3	1:A:372:VAL:HG22	1.85	0.58
1:A:134:PHE:HE1	1:A:193:MET:HE3	1.69	0.58
1:A:498:GLN:HG2	1:A:526:LEU:HD23	1.88	0.56
1:A:1008:ARG:HB3	1:A:1042:SER:HB2	1.88	0.55
1:A:558:HIS:HB3	1:A:930:ASP:HB2	1.88	0.55
1:A:777:ARG:HG2	1:A:891:ILE:HG22	1.88	0.55
1:A:686:LEU:HD21	1:A:774:PRO:HG3	1.89	0.55
1:A:216:LEU:O	1:A:221:PHE:HB2	2.07	0.54
1:A:1010:GLU:OE1	1:A:1022:HIS:HA	2.08	0.53
1:A:426:LYS:HD3	1:A:851:PRO:O	2.09	0.52
1:A:134:PHE:CE1	1:A:193:MET:HE3	2.43	0.52
1:A:1010:GLU:CD	1:A:1022:HIS:HD1	2.18	0.52
1:A:70:TYR:HB3	1:A:327:GLU:HG2	1.91	0.52
1:A:421:SER:O	1:A:426:LYS:NZ	2.43	0.51
1:A:572:TYR:OH	2:A:1102:PEG:H21	2.11	0.50
1:A:652:LEU:HD11	1:A:676:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:ILE:HB	1:A:892:TYR:HB2	1.92	0.50
1:A:753:GLU:HG3	1:A:770:ARG:HG2	1.94	0.50
1:A:804:PHE:CG	1:A:856:SER:HB3	2.47	0.50
1:A:93:PRO:HD2	1:A:470:HIS:CE1	2.47	0.49
1:A:601:ASP:OD1	1:A:608:HIS:NE2	2.46	0.49
1:A:419:TYR:CZ	1:A:830:PRO:HD3	2.48	0.49
1:A:555:VAL:HG23	1:A:557:MET:HE1	1.94	0.48
1:A:629:LEU:HD12	1:A:946:PHE:HB3	1.95	0.48
1:A:344:PHE:HB3	1:A:350:TRP:NE1	2.29	0.47
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.49	0.47
1:A:804:PHE:CD1	1:A:856:SER:HB3	2.49	0.47
1:A:1010:GLU:OE2	1:A:1022:HIS:CE1	2.66	0.47
1:A:170:GLU:CD	1:A:212:MET:HG3	2.41	0.46
1:A:68:ILE:HD12	1:A:277:PRO:HG3	1.96	0.46
1:A:530:ARG:HG2	1:A:530:ARG:HH11	1.80	0.46
1:A:592:VAL:HA	1:A:617:ARG:O	2.16	0.46
1:A:244:GLU:OE2	1:A:382:TYR:OH	2.30	0.46
1:A:180:LEU:HD22	1:A:465:LEU:HD23	1.98	0.45
1:A:82:LYS:HD2	1:A:373:GLN:HB3	1.98	0.45
1:A:832:PRO:HA	1:A:851:PRO:HB3	1.99	0.45
1:A:595:VAL:HG11	1:A:615:LYS:HE3	2.00	0.44
1:A:599:HIS:CD2	1:A:608:HIS:NE2	2.84	0.44
1:A:715:TYR:HB2	1:A:789:GLU:HB2	1.99	0.44
1:A:968:SER:C	1:A:970:ALA:H	2.26	0.44
1:A:840:ALA:HA	1:A:904:ARG:HH22	1.83	0.44
1:A:838:GLU:CD	1:A:904:ARG:HH11	2.26	0.43
1:A:358:GLU:O	1:A:362:GLU:HB2	2.18	0.43
1:A:869:ARG:C	1:A:870:LEU:HG	2.43	0.43
1:A:94:GLY:HA2	1:A:97:GLN:O	2.18	0.43
1:A:344:PHE:HB3	1:A:350:TRP:CE2	2.53	0.43
1:A:335:LEU:HB2	1:A:382:TYR:CD1	2.53	0.43
1:A:45:MET:HB2	1:A:402:GLY:HA3	2.02	0.42
1:A:792:MET:O	1:A:863:GLU:HA	2.20	0.42
1:A:570:ASP:HA	1:A:618:ILE:O	2.20	0.42
1:A:582:ASP:OD1	1:A:584:ALA:HB3	2.20	0.42
1:A:777:ARG:HB3	1:A:889:LEU:HD11	2.01	0.42
1:A:100:GLU:O	1:A:104:GLN:HG2	2.19	0.41
1:A:116:ARG:NH2	1:A:347:ASN:HD21	2.18	0.41
1:A:403:ASP:CG	1:A:816:ARG:HH12	2.28	0.41
1:A:566:GLU:HA	1:A:622:ALA:O	2.20	0.41
1:A:408:ALA:HA	1:A:413:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:HIS:HE1	1:A:560:THR:HG21	1.86	0.41
1:A:804:PHE:HB3	1:A:856:SER:HB3	2.03	0.41
1:A:755:SER:HA	1:A:767:THR:O	2.21	0.40
1:A:307:SER:O	1:A:311:VAL:HB	2.22	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	996/1033 (96%)	940 (94%)	50 (5%)	6 (1%)	21 35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TRP
1	A	762	SER
1	A	122	PRO
1	A	655	ASN
1	A	272	PRO
1	A	783	GLY

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	852/918 (93%)	820 (96%)	32 (4%)	29 53

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	61	VAL
1	A	122	PRO
1	A	144	ASN
1	A	206	PHE
1	A	236	GLU
1	A	241	ARG
1	A	275	CYS
1	A	290	MET
1	A	295	LEU
1	A	317	LEU
1	A	327	GLU
1	A	410	ARG
1	A	537	GLU
1	A	589	GLU
1	A	604	THR
1	A	606	THR
1	A	658	SER
1	A	659	LEU
1	A	675	GLU
1	A	682	ASN
1	A	702	ASP
1	A	738	VAL
1	A	760	LEU
1	A	776	ILE
1	A	788	THR
1	A	807	ASP
1	A	831	ILE
1	A	842	THR
1	A	895	VAL
1	A	998	ASP
1	A	1018	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS

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Mol	Chain	Res	Type
1	A	191	GLN
1	A	223	ASN
1	A	347	ASN
1	A	388	GLN
1	A	554	HIS
1	A	567	GLN
1	A	599	HIS
1	A	600	HIS
1	A	610	GLN
1	A	698	GLN
1	A	732	ASN
1	A	919	HIS
1	A	1005	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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	PEG	A	1102	-	6,6,6	0.20	0	5,5,5	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1IGC	A	1103	4	13,13,20	0.75	0	14,19,27	1.41	2 (14%)
2	PEG	A	1101	-	6,6,6	0.27	0	5,5,5	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	PEG	A	1102	-	-	4/4/4/4	-
3	A1IGC	A	1103	4	-	-	0/2/2/2
2	PEG	A	1101	-	-	3/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1103	A1IGC	O1-C9-C10	-3.93	103.69	111.43
3	A	1103	A1IGC	O2-C10-C9	-2.38	106.32	111.97

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	PEG	O1-C1-C2-O2
2	A	1102	PEG	O1-C1-C2-O2
2	A	1102	PEG	C4-C3-O2-C2
2	A	1102	PEG	O2-C3-C4-O4
2	A	1101	PEG	O2-C3-C4-O4
2	A	1102	PEG	C1-C2-O2-C3
2	A	1101	PEG	C1-C2-O2-C3

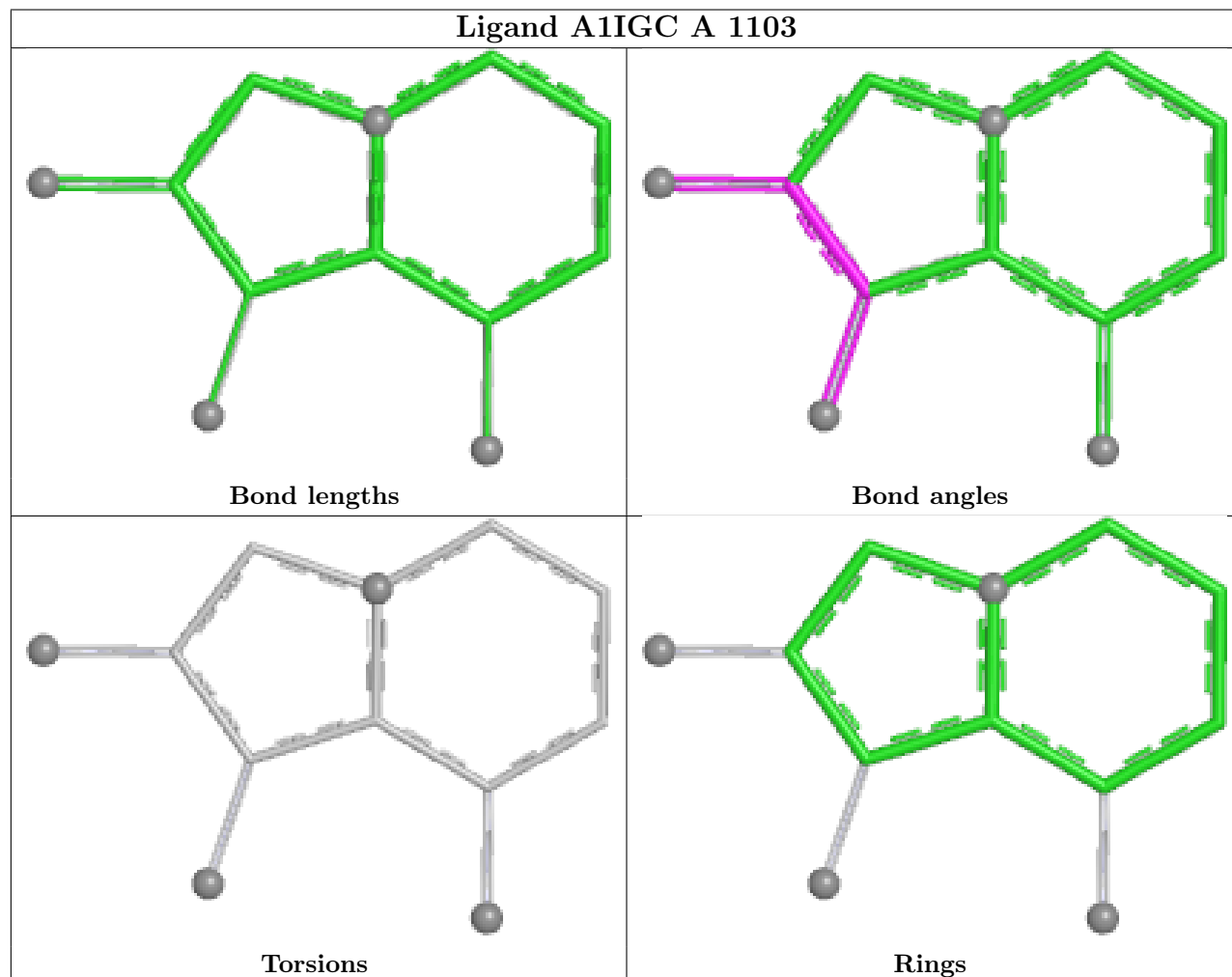
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1102	PEG	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	1006/1033 (97%)	-0.09	12 (1%) 76 74	25, 49, 86, 141	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	PHE	3.5
1	A	903	VAL	2.8
1	A	740	LEU	2.8
1	A	712	PHE	2.5
1	A	659	LEU	2.4
1	A	760	LEU	2.4
1	A	658	SER	2.3
1	A	603	LEU	2.3
1	A	294	GLY	2.2
1	A	607	ILE	2.2
1	A	761	PRO	2.2
1	A	878	LEU	2.1

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,

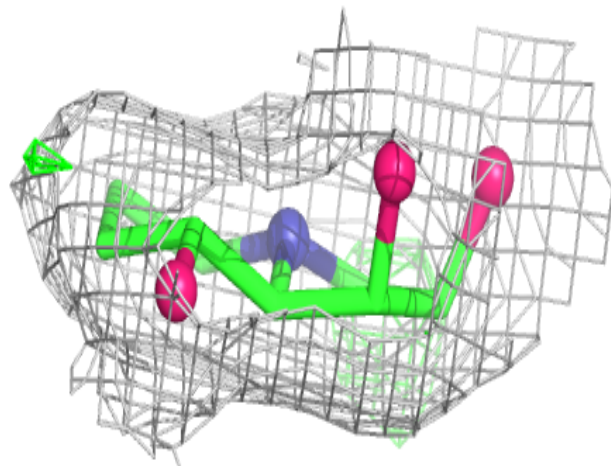
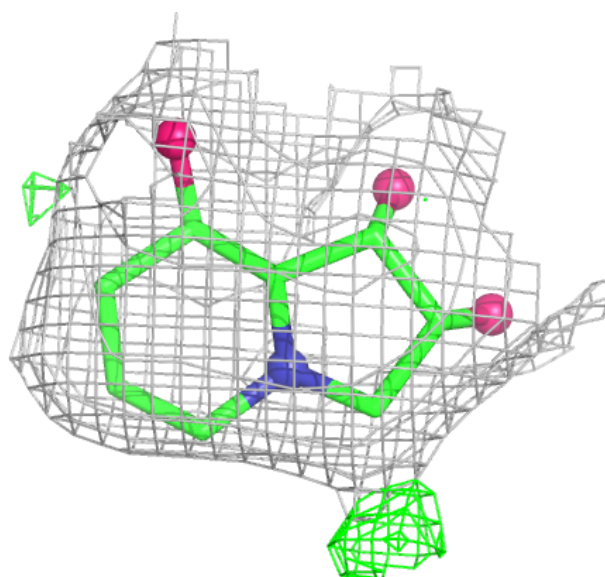
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PEG	A	1101	7/7	0.81	0.13	71,74,79,80	0
2	PEG	A	1102	7/7	0.82	0.12	71,75,81,83	0
3	A1IGC	A	1103	12/19	0.93	0.08	34,37,44,50	0
4	ZN	A	1104	1/1	0.99	0.02	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 A1IGC A 1103:

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.