Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:24 PM UTC

PDB ID	:	6RRX / pdb_00006rrx
Title	:	GOLGI ALPHA-MANNOSIDASE II in complex with (2S,3R)-2-(Hydroxymethyl)-3-piperidinol
Authors	:	Armstrong, Z.; Lahav, D.; Johnson, R.; Kuo, C.L.; Beenakker, T.J.M.; de Boer, C.; Wong, C.S.; van Rijssel, E.R.; Debets, M.; Geurink, P.P.; Ovaa, H.; van der Stelt, M.; Codee, J.D.C.; Aerts, J.M.F.G.; Wu, L.; Overkleeft, H.S.; Davies, G.J.
Deposited on	:	2019-05-20
Resolution	:	1.84 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:

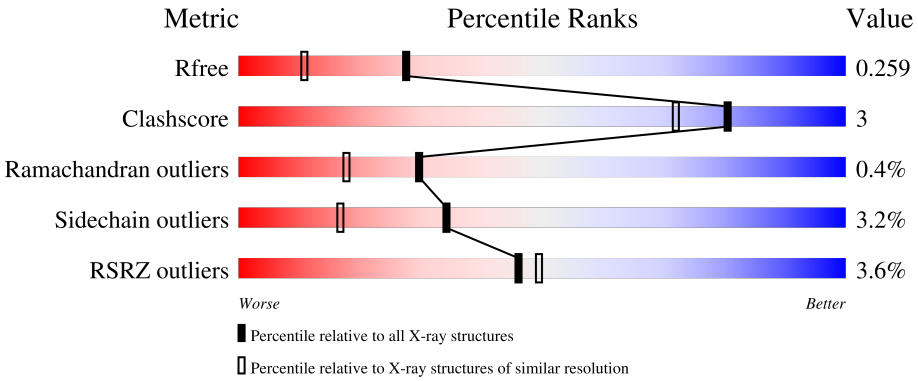
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

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 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	1033	3% 87% 9% .

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8453 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.

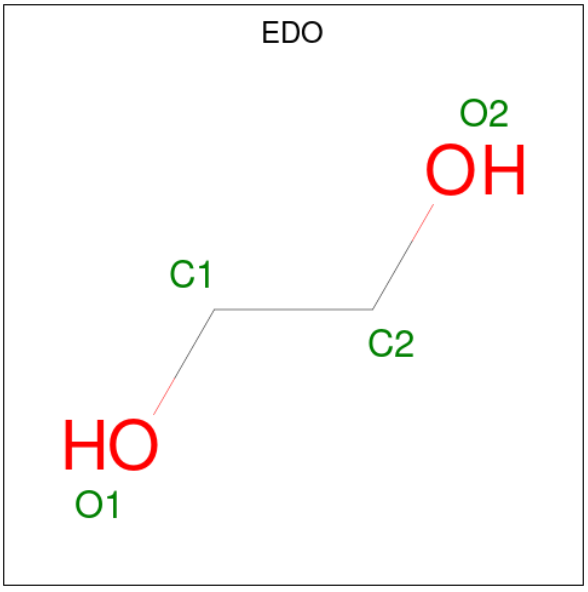
- Molecule 1 is a protein called Alpha-mannosidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	9	0
			8087	5146	1418	1483	40			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

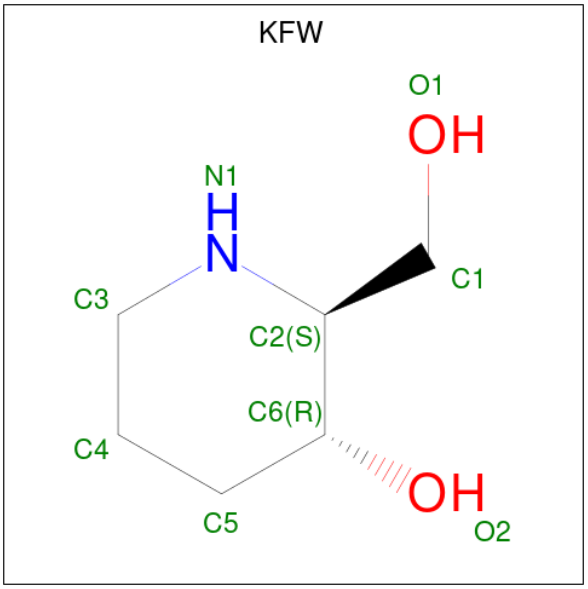
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- 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		

- Molecule 4 is (2 {S},3 {R})-2-(hydroxymethyl)piperidin-3-ol (CCD ID: KFW) (formula: $C_6H_{13}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 9 6 1 2	0	0

- Molecule 5 is water.

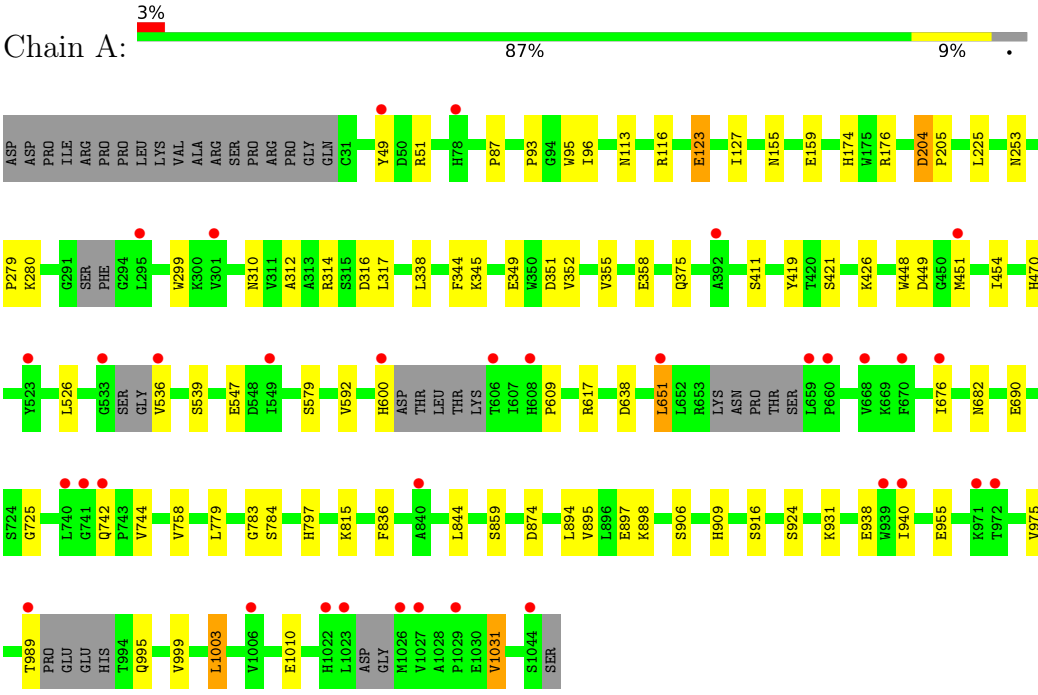
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	348	Total O 348 348	0	0

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: Alpha-mannosidase 2

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.00Å 91.38Å 132.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.34 – 1.84 75.23 – 1.84	Depositor EDS
% Data completeness (in resolution range)	100.0 (75.34-1.84) 100.0 (75.23-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.200 , 0.256 0.208 , 0.259	Depositor DCC
R_{free} test set	4689 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.671	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 32.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8453	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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, ZN, KFW

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	1.03	0/8318	1.32	10/11285 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	836	PHE	CA-CB-CG	5.84	119.64	113.80
1	A	123	GLU	CB-CG-CD	5.82	122.49	112.60
1	A	797	HIS	N-CA-C	-5.78	106.14	112.72
1	A	316	ASP	CA-C-N	5.28	127.31	120.44
1	A	316	ASP	C-N-CA	5.28	127.31	120.44
1	A	421	SER	CA-C-N	5.25	128.50	122.83
1	A	421	SER	C-N-CA	5.25	128.50	122.83
1	A	638	ASP	CB-CA-C	-5.21	102.47	110.81
1	A	253	ASN	CA-C-N	5.00	129.13	120.58
1	A	253	ASN	C-N-CA	5.00	129.13	120.58

There are no chirality outliers.

There are no planarity outliers.

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	8087	0	7889	41	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	8	0	12	0	0
4	A	9	0	0	0	0
5	A	348	0	0	3	0
All	All	8453	0	7901	41	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 3.

All (41) 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:916:SER:OG	1:A:955:GLU:OE1	2.21	0.57
1:A:498:GLN:HG2	1:A:526:LEU:HD12	1.88	0.56
1:A:844:LEU:HD11	1:A:894:LEU:HD11	1.90	0.54
1:A:375:GLN:NE2	5:A:1215:HOH:O	2.42	0.52
1:A:174:HIS:CE1	1:A:176:ARG:HD3	2.44	0.52
1:A:123:GLU:OE2	1:A:358:GLU:OE2	2.30	0.50
1:A:96:ILE:HG23	1:A:479:LYS:HE2	1.94	0.49
1:A:719:SER:O	1:A:723:ARG:NH2	2.40	0.49
1:A:981[B]:ARG:HH11	1:A:981[B]:ARG:HG3	1.78	0.49
1:A:312:ALA:HB3	5:A:1467:HOH:O	2.14	0.48
1:A:815[A]:LYS:HE3	1:A:909:HIS:O	2.13	0.48
1:A:536:VAL:HG22	1:A:779:LEU:CD1	2.44	0.47
1:A:498:GLN:HG2	1:A:526:LEU:CD1	2.45	0.47
1:A:592:VAL:HA	1:A:617:ARG:O	2.14	0.47
1:A:113:ASN:ND2	1:A:345:LYS:O	2.47	0.47
1:A:526:LEU:HD23	1:A:931:LYS:O	2.15	0.47
1:A:314:ARG:NH1	5:A:1206:HOH:O	2.36	0.46
1:A:979:LEU:HD21	1:A:999:VAL:HG11	1.97	0.46
1:A:815[A]:LYS:NZ	1:A:909:HIS:O	2.46	0.46
1:A:344:PHE:H	1:A:349:GLU:CD	2.23	0.46
1:A:449:ASP:OD2	1:A:451:MET:HB2	2.17	0.45
1:A:225:LEU:HD21	1:A:264[A]:MET:SD	2.57	0.45
1:A:279:PRO:HB2	1:A:299:TRP:CZ2	2.52	0.44
1:A:981[B]:ARG:HG3	1:A:981[B]:ARG:NH1	2.32	0.44
1:A:310:ASN:OD1	1:A:310:ASN:C	2.61	0.43
1:A:975:VAL:HG21	1:A:1003:LEU:CD2	2.49	0.43
1:A:127:ILE:HA	1:A:159:GLU:O	2.19	0.42
1:A:651:LEU:HD23	1:A:651:LEU:HA	1.90	0.42
1:A:895:VAL:HG12	1:A:897:GLU:HG3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:TRP:CG	1:A:454:ILE:HG13	2.56	0.41
1:A:93:PRO:HD2	1:A:470:HIS:CE1	2.56	0.41
1:A:280:LYS:HG3	1:A:299:TRP:HB3	2.01	0.41
1:A:609:PRO:CD	1:A:744:VAL:HG11	2.51	0.41
1:A:981[B]:ARG:NE	1:A:1031:VAL:O	2.47	0.41
1:A:419:TYR:C	1:A:426:LYS:HE2	2.46	0.40
1:A:204:ASP:H	1:A:205:PRO:HD3	1.86	0.40
1:A:351:ASP:O	1:A:355:VAL:HG23	2.22	0.40
1:A:725:GLY:HA3	1:A:874:ASP:CG	2.45	0.40
1:A:87:PRO:HA	1:A:338:LEU:O	2.21	0.40
1:A:155:ASN:OD1	1:A:155:ASN:C	2.64	0.40
1:A:975:VAL:HG21	1:A:1003:LEU:HD23	2.03	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	989/1033 (96%)	956 (97%)	29 (3%)	4 (0%)	30 18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TRP
1	A	411	SER
1	A	783	GLY
1	A	204	ASP

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	892/918 (97%)	864 (97%)	28 (3%)	35 18

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	TYR
1	A	51	ARG
1	A	116	ARG
1	A	275	CYS
1	A	317	LEU
1	A	352	VAL
1	A	539	SER
1	A	547	GLU
1	A	579	SER
1	A	600	HIS
1	A	651	LEU
1	A	676	ILE
1	A	682	ASN
1	A	690	GLU
1	A	742	GLN
1	A	758	VAL
1	A	784	SER
1	A	859	SER
1	A	898	LYS
1	A	906	SER
1	A	924	SER
1	A	938	GLU
1	A	940	ILE
1	A	989	THR
1	A	995	GLN
1	A	1003	LEU
1	A	1010	GLU
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	44	GLN
1	A	144	ASN
1	A	249	GLN
1	A	371	ASN
1	A	373	GLN
1	A	394	GLN
1	A	608	HIS
1	A	610	GLN
1	A	720	HIS
1	A	778	ASN
1	A	797	HIS
1	A	809	ASN
1	A	812	GLN
1	A	866	GLN
1	A	919	HIS

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	$\#\|Z\|>2$
4	KFW	A	1103	2	9,9,9	0.41	0	9,11,11	1.19	1 (11%)
3	EDO	A	1104	-	3,3,3	0.05	0	2,2,2	0.06	0
3	EDO	A	1102	-	3,3,3	0.19	0	2,2,2	0.19	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
4	KFW	A	1103	2	-	0/2/13/13	0/1/1/1
3	EDO	A	1104	-	-	0/1/1/1	-
3	EDO	A	1102	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1103	KFW	C3-N1-C2	3.11	113.56	111.62

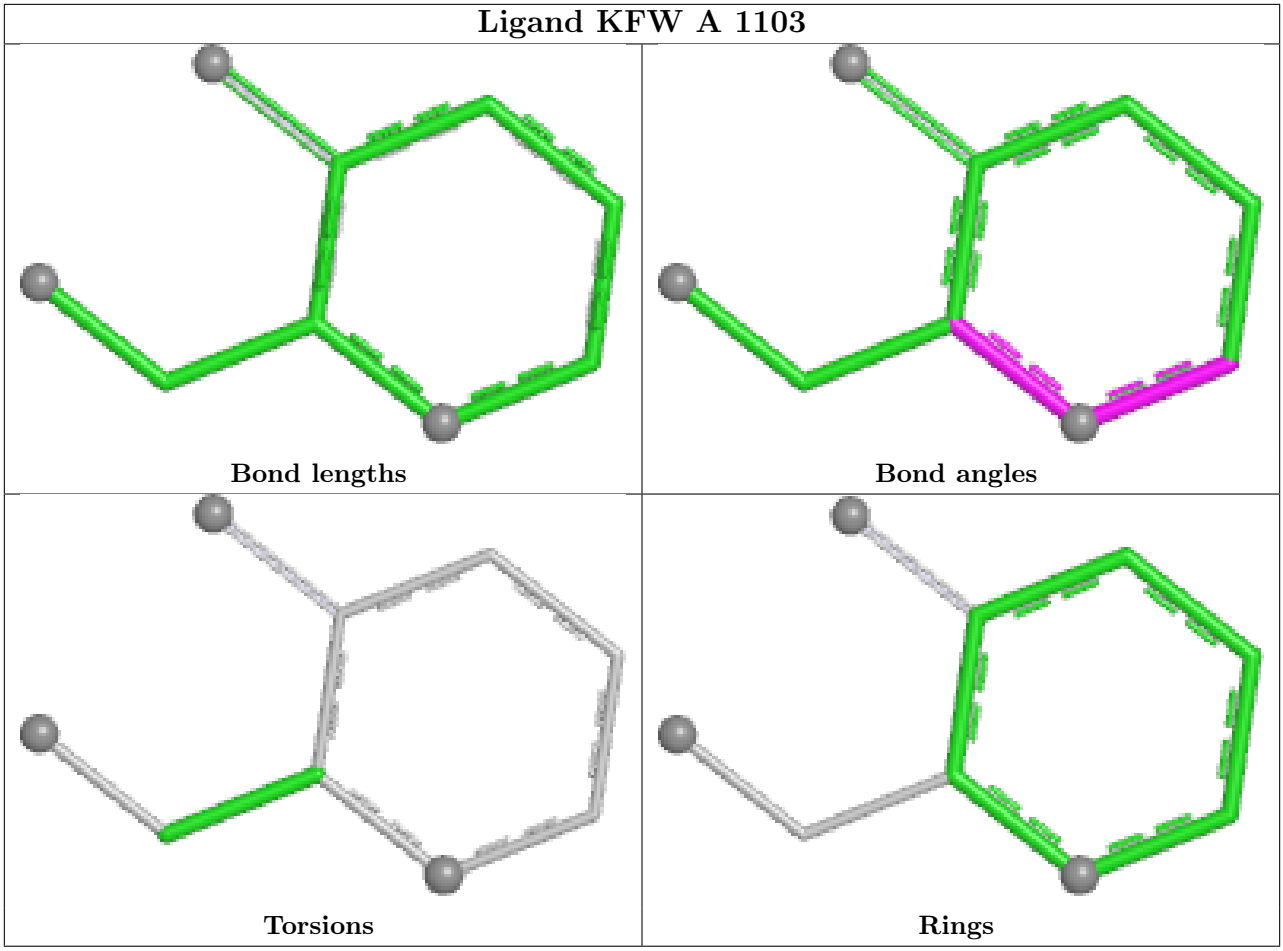
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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.



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	994/1033 (96%)	0.38	36 (3%) 46 49	15, 42, 69, 95	9 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	659	LEU	4.1
1	A	536	VAL	3.5
1	A	676	ILE	3.4
1	A	940	ILE	3.4
1	A	1023	LEU	3.4
1	A	49	TYR	3.1
1	A	741	GLY	3.1
1	A	549	ILE	2.7
1	A	989	THR	2.7
1	A	295	LEU	2.7
1	A	78	HIS	2.5
1	A	451	MET	2.5
1	A	1022	HIS	2.4
1	A	1026	MET	2.4
1	A	660	PRO	2.4
1	A	1044	SER	2.4
1	A	668	VAL	2.3
1	A	651	LEU	2.2
1	A	1027	VAL	2.2
1	A	740	LEU	2.2
1	A	523	TYR	2.1
1	A	600	HIS	2.1
1	A	840	ALA	2.1
1	A	670	PHE	2.1
1	A	939	TRP	2.1
1	A	392	ALA	2.1
1	A	742	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1006	VAL	2.1
1	A	1029	PRO	2.1
1	A	533	GLY	2.0
1	A	608	HIS	2.0
1	A	301	VAL	2.0
1	A	971	LYS	2.0
1	A	720	HIS	2.0
1	A	606	THR	2.0
1	A	972	THR	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)

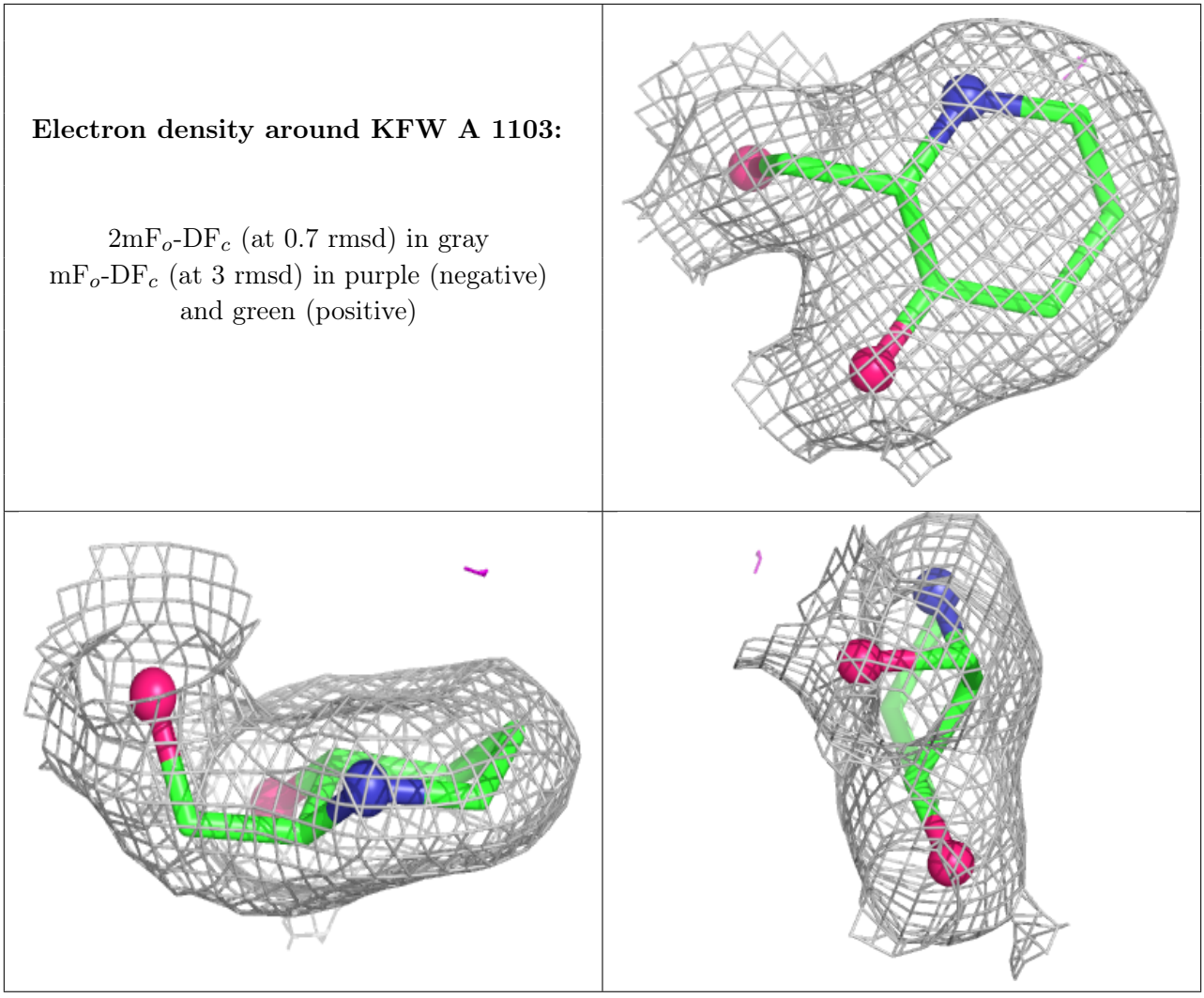
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	EDO	A	1104	4/4	0.91	0.12	44,49,50,56	0
3	EDO	A	1102	4/4	0.92	0.11	36,38,38,42	0
4	KFW	A	1103	9/9	0.96	0.06	30,33,36,37	0
2	ZN	A	1101	1/1	0.99	0.02	30,30,30,30	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 KFW 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

There are no such residues in this entry.