



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:31 PM UTC

PDB ID : 8RMI / pdb_00008rmi
Title : Crystal structure of ferrioxamine transporter FoxA
Authors : Josts, I.; Tidow, H.; Mislin, G.
Deposited on : 2024-01-06
Resolution : 2.48 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

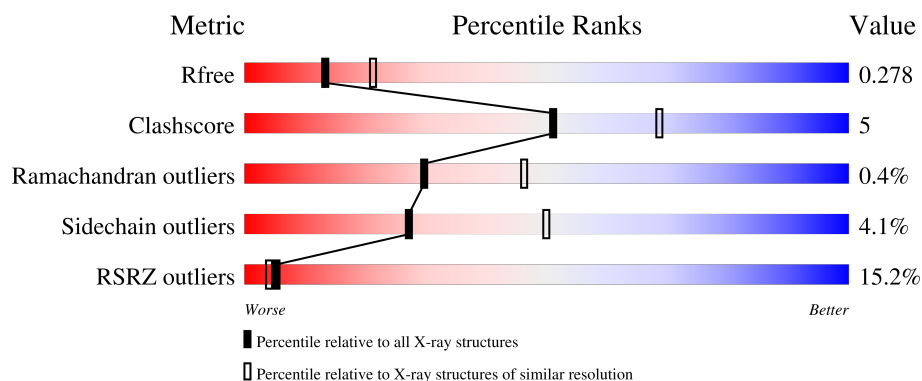
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	820	13% 71% 10% • 17%

2 Entry composition [i](#)

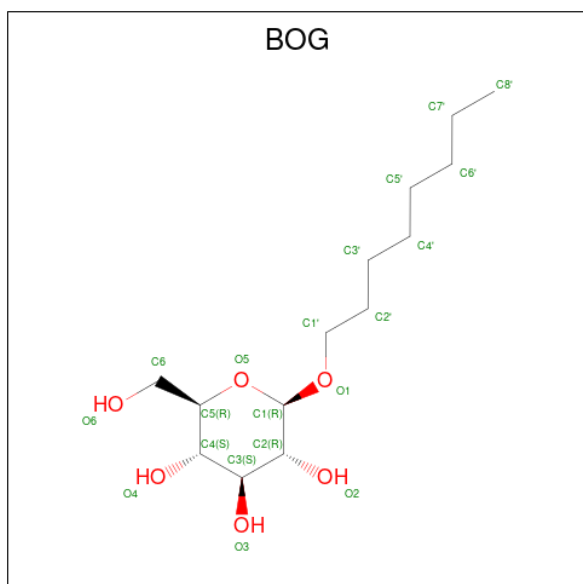
There are 9 unique types of molecules in this entry. The entry contains 5519 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ferrioxamine receptor FoxA.

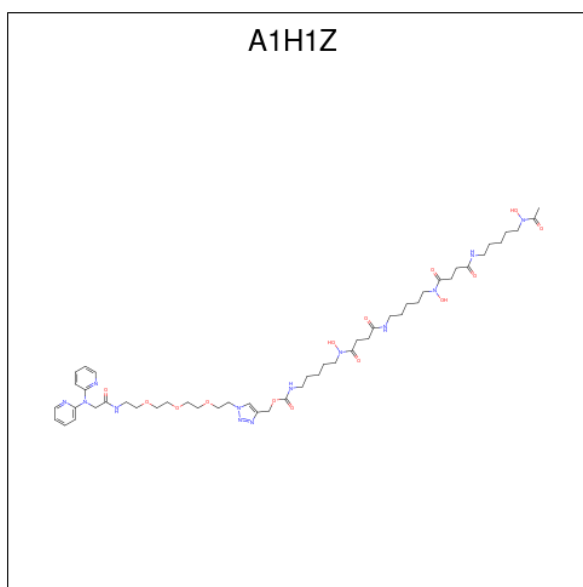
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	677	5325	3345	910	1059	11	0	0	0

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



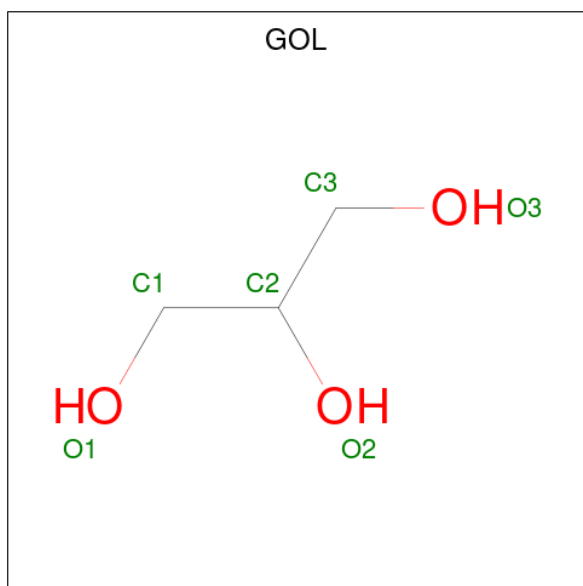
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	20	14	6	0	0
2	A	1	20	14	6	0	0

- Molecule 3 is [1-[2-[2-[2-[2-[2-(dipyridin-2-ylamino)ethanoylamino]ethoxy]ethoxy]ethoxy]ethyl]-1,2,3-triazol-4-yl]methyl {N}-[5-[[4-[5-[[4-[5-[ethanoyl(oxidanyl)amino]pentylamino]-4-oxidanylidene-butanoyl]-oxidanyl-amino]pentylamino]-4-oxidanylidene-butanoyl]-oxidanyl-amino]pentyl]carbamate (CCD ID: A1H1Z) (formula: C₄₉H₇₇N₁₃O₁₄) (labeled as "Ligand of Interest" by depositor).



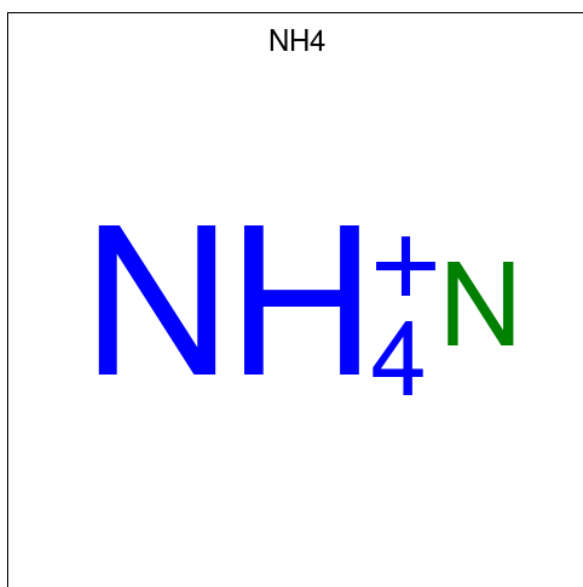
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			76	49	13	14		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is AMMONIUM ION (CCD ID: NH4) (formula: H_4N).

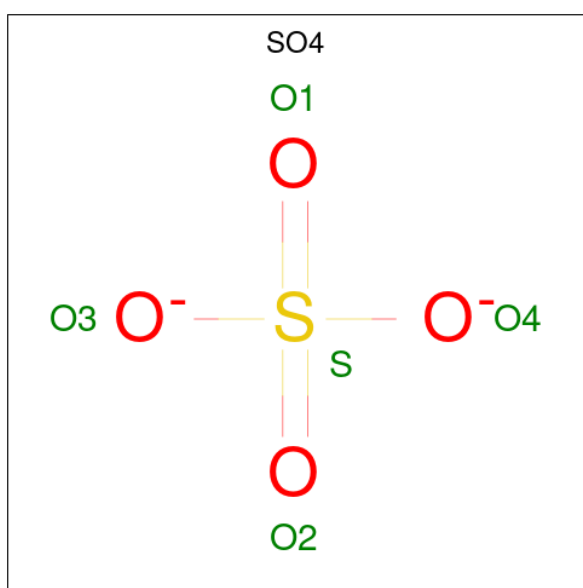


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total N 1 1	0	0

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Fe 1 1	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Na 1 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	39	Total O 39 39	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.52Å 93.52Å 177.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.99 – 2.48 80.99 – 2.48	Depositor EDS
% Data completeness (in resolution range)	50.4 (80.99-2.48) 50.4 (80.99-2.48)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.219 , 0.268 0.234 , 0.278	Depositor DCC
R_{free} test set	845 reflections (2.59%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5519	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: A1H1Z, FE, NH4, NA, GOL, SO4, BOG

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	0.68	2/5451 (0.0%)	1.17	21/7397 (0.3%)

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	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	662	ASN	CA-C	5.51	1.58	1.53
1	A	367	HIS	CG-CD2	-5.14	1.30	1.35

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	LYS	N-CA-C	-11.80	94.42	111.30
1	A	397	ASP	CA-CB-CG	8.55	121.15	112.60
1	A	301	MET	CG-SD-CE	8.35	119.27	100.90
1	A	663	PHE	CA-CB-CG	7.92	121.72	113.80
1	A	663	PHE	N-CA-C	7.84	121.87	110.42
1	A	389	ARG	N-CA-C	-7.49	103.44	112.58
1	A	661	ASP	CA-CB-CG	7.47	120.07	112.60
1	A	395	PHE	CA-CB-CG	7.41	121.21	113.80
1	A	390	HIS	CA-CB-CG	7.04	120.83	113.80
1	A	332	ASP	N-CA-C	-6.70	101.89	110.53
1	A	613	ASP	CA-CB-CG	6.51	119.11	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	MET	CG-SD-CE	6.27	114.70	100.90
1	A	685	ASP	N-CA-C	-6.26	104.21	113.72
1	A	355	ASP	N-CA-C	-6.00	105.72	113.16
1	A	521	ASP	CB-CA-C	-5.15	102.72	111.02
1	A	422	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	221	MET	CG-SD-CE	-5.13	89.62	100.90
1	A	380	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	400	PRO	N-CA-C	-5.09	101.99	112.47
1	A	585	ARG	CG-CD-NE	5.07	123.14	112.00
1	A	207	THR	CA-CB-CG2	5.06	119.11	110.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331	SER	Peptide
1	A	389	ARG	Sidechain
1	A	463	ARG	Sidechain
1	A	496	ARG	Sidechain
1	A	585	ARG	Sidechain

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	5325	0	5038	54	0
2	A	40	0	56	0	0
3	A	76	0	0	1	0
4	A	6	0	8	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	30	0	0	0	0
8	A	1	0	0	0	0
9	A	39	0	0	6	0
All	All	5519	0	5102	55	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 5.

All (55) 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:399:GLU:CG	1:A:442:VAL:O	1.77	1.33
1:A:399:GLU:OE2	1:A:441:GLN:CG	2.02	1.07
1:A:399:GLU:OE2	1:A:441:GLN:HG3	1.54	1.07
1:A:399:GLU:HG2	1:A:442:VAL:O	0.89	1.05
1:A:399:GLU:HG2	1:A:442:VAL:C	2.03	0.79
1:A:399:GLU:OE2	1:A:441:GLN:HG2	1.82	0.78
1:A:199:MET:HE1	1:A:259:ILE:HG21	1.73	0.70
1:A:400:PRO:HD3	1:A:442:VAL:HB	1.73	0.69
1:A:395:PHE:O	9:A:1001:HOH:O	2.09	0.69
1:A:683:LEU:O	1:A:685:ASP:N	2.27	0.67
1:A:153:SER:OG	1:A:160:THR:HG21	1.95	0.67
1:A:336:ASP:N	9:A:1001:HOH:O	2.28	0.64
1:A:399:GLU:CD	1:A:441:GLN:HG3	2.26	0.60
1:A:387:ASN:C	1:A:389:ARG:H	2.11	0.58
1:A:152:GLY:CA	1:A:161:HIS:HB2	2.35	0.57
1:A:387:ASN:O	1:A:389:ARG:N	2.37	0.57
1:A:153:SER:OG	1:A:160:THR:CG2	2.53	0.56
1:A:684:SER:C	1:A:686:ASN:H	2.13	0.56
1:A:397:ASP:HB2	9:A:1001:HOH:O	2.05	0.55
1:A:555:LEU:HD23	1:A:586:ILE:HG13	1.89	0.55
1:A:297:SER:O	1:A:298:ILE:HD13	2.05	0.55
1:A:331:SER:OG	1:A:332:ASP:O	2.17	0.53
1:A:165:ALA:O	1:A:585:ARG:NH2	2.41	0.52
1:A:387:ASN:C	1:A:389:ARG:N	2.68	0.51
1:A:389:ARG:NE	1:A:389:ARG:HA	2.24	0.51
1:A:684:SER:O	1:A:685:ASP:HB3	2.10	0.51
1:A:767:ARG:O	1:A:768:ILE:HD12	2.11	0.51
1:A:399:GLU:CD	1:A:442:VAL:O	2.52	0.50
1:A:739:GLY:HA3	9:A:1002:HOH:O	2.10	0.50
1:A:205:ILE:O	1:A:719:MET:HE1	2.12	0.49
1:A:723:TRP:CE2	9:A:1002:HOH:O	2.66	0.49
1:A:221:MET:CE	1:A:279:VAL:HG23	2.43	0.48
1:A:161:HIS:CD2	1:A:171:PRO:HA	2.49	0.48
1:A:436:ASP:OD1	1:A:463:ARG:NH2	2.47	0.47
1:A:221:MET:HE1	1:A:279:VAL:HG23	1.97	0.47
1:A:421:ASP:HB3	1:A:423:VAL:H	1.79	0.47
1:A:355:ASP:O	1:A:419:ARG:NH1	2.49	0.46
1:A:738:ILE:HG22	1:A:768:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:TYR:CZ	1:A:238:LYS:HD3	2.53	0.44
1:A:421:ASP:HB2	1:A:424:TRP:H	1.82	0.44
1:A:781:ASP:OD1	1:A:817:ASN:HB2	2.17	0.44
1:A:684:SER:C	1:A:686:ASN:N	2.72	0.43
1:A:400:PRO:HD3	1:A:442:VAL:CB	2.46	0.43
1:A:512:ASP:OD1	1:A:514:PHE:O	2.36	0.43
3:A:903:A1H1Z:O07	3:A:903:A1H1Z:N06	2.51	0.43
1:A:193:LYS:HE3	1:A:813:THR:HG21	2.01	0.42
1:A:210:VAL:HG12	1:A:210:VAL:O	2.19	0.42
1:A:637:GLY:O	1:A:638:SER:C	2.62	0.42
1:A:600:VAL:HG22	1:A:629:LEU:HD23	2.02	0.42
1:A:794:TYR:CZ	1:A:807:GLY:HA3	2.55	0.42
1:A:686:ASN:HB3	1:A:727:ALA:O	2.20	0.41
1:A:199:MET:HB3	1:A:205:ILE:HG21	2.03	0.41
1:A:152:GLY:HA2	1:A:161:HIS:HB2	2.02	0.41
1:A:511:LEU:HD12	9:A:1019:HOH:O	2.20	0.40
1:A:586:ILE:HG22	1:A:602:TYR:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	675/820 (82%)	650 (96%)	22 (3%)	3 (0%)	30	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	387	ASN
1	A	684	SER
1	A	388	GLY

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	566/667 (85%)	543 (96%)	23 (4%)	27	50

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	LEU
1	A	249	MET
1	A	389	ARG
1	A	403	ASP
1	A	404	ASP
1	A	499	THR
1	A	504	ARG
1	A	514	PHE
1	A	527	PRO
1	A	557	LEU
1	A	576	ASP
1	A	577	ASP
1	A	617	THR
1	A	629	LEU
1	A	660	GLN
1	A	689	LEU
1	A	734	SER
1	A	748	THR
1	A	768	ILE
1	A	774	LYS
1	A	777	LEU
1	A	785	ASN
1	A	816	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	A	293	GLN

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Mol	Chain	Res	Type
1	A	362	GLN
1	A	370	ASN
1	A	543	GLN
1	A	648	HIS
1	A	673	GLN
1	A	714	GLN

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 13 ligands modelled in this entry, 1 is modelled with single atom and 2 are monoatomic - leaving 10 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	$\# Z > 2$
7	SO4	A	911	-	4,4,4	0.31	0	6,6,6	0.10	0
7	SO4	A	910	-	4,4,4	0.21	0	6,6,6	0.25	0
2	BOG	A	901	-	20,20,20	0.59	0	25,25,25	1.18	3 (12%)
3	A1H1Z	A	903	6	77,78,78	2.37	18 (23%)	83,95,95	3.00	37 (44%)
7	SO4	A	907	-	4,4,4	0.33	0	6,6,6	0.20	0
7	SO4	A	909	-	4,4,4	0.28	0	6,6,6	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	904	-	5,5,5	0.20	0	5,5,5	0.51	0
7	SO4	A	912	-	4,4,4	0.37	0	6,6,6	0.41	0
2	BOG	A	902	-	20,20,20	0.69	0	25,25,25	0.90	1 (4%)
7	SO4	A	908	-	4,4,4	0.33	0	6,6,6	0.14	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	GOL	A	904	-	-	2/4/4/4	-
2	BOG	A	901	-	-	9/11/31/31	0/1/1/1
2	BOG	A	902	-	-	4/11/31/31	0/1/1/1
3	A1H1Z	A	903	6	-	44/81/81/81	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	A1H1Z	C05-N01	7.35	1.45	1.35
3	A	903	A1H1Z	C25-N06	6.23	1.47	1.34
3	A	903	A1H1Z	C40-N11	6.07	1.53	1.40
3	A	903	A1H1Z	C17-N04	6.03	1.47	1.33
3	A	903	A1H1Z	C08-N02	5.73	1.47	1.33
3	A	903	A1H1Z	C41-N11	5.40	1.51	1.40
3	A	903	A1H1Z	C29-C28	4.60	1.44	1.36
3	A	903	A1H1Z	C38-N10	4.33	1.43	1.33
3	A	903	A1H1Z	C14-N03	4.21	1.40	1.35
3	A	903	A1H1Z	C07-C08	4.15	1.59	1.51
3	A	903	A1H1Z	O01-C25	3.76	1.42	1.35
3	A	903	A1H1Z	O08-N01	-3.75	1.37	1.40
3	A	903	A1H1Z	O09-N03	-3.62	1.37	1.40
3	A	903	A1H1Z	O07-C14	-3.38	1.15	1.23
3	A	903	A1H1Z	C27-C28	3.03	1.54	1.49
3	A	903	A1H1Z	O14-C38	-2.76	1.17	1.23
3	A	903	A1H1Z	C46-C40	2.36	1.44	1.39
3	A	903	A1H1Z	C13-N03	-2.14	1.43	1.46

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	903	A1H1Z	C06-C07-C08	11.41	136.15	112.67
3	A	903	A1H1Z	C42-N12-C41	7.74	128.06	116.81
3	A	903	A1H1Z	O01-C25-N06	6.75	121.75	110.62
3	A	903	A1H1Z	C16-C17-N04	6.28	127.79	116.34
3	A	903	A1H1Z	O06-C08-N02	-5.96	111.34	123.03
3	A	903	A1H1Z	N09-N08-N07	4.95	111.47	107.02
3	A	903	A1H1Z	C27-C28-N07	4.83	129.49	121.49
3	A	903	A1H1Z	C07-C08-N02	4.82	125.13	116.34
3	A	903	A1H1Z	C21-C22-N05	4.79	120.98	111.11
3	A	903	A1H1Z	C49-N13-C40	4.39	123.19	116.81
3	A	903	A1H1Z	O02-C25-N06	-4.33	118.41	124.93
3	A	903	A1H1Z	O09-N03-C13	4.30	123.84	113.76
3	A	903	A1H1Z	C27-O01-C25	4.24	120.59	115.67
3	A	903	A1H1Z	C45-C41-N12	-4.06	115.45	123.46
3	A	903	A1H1Z	C10-C09-N02	-3.87	101.34	112.20
3	A	903	A1H1Z	C03-C04-N01	3.72	118.77	111.11
3	A	903	A1H1Z	O04-C17-C16	-3.70	115.32	122.02
3	A	903	A1H1Z	C15-C16-C17	3.65	120.18	112.67
3	A	903	A1H1Z	C30-N09-N08	3.61	128.04	120.78
3	A	903	A1H1Z	C43-C42-N12	-3.61	117.71	123.42
3	A	903	A1H1Z	C27-C28-C29	-3.52	124.15	130.22
3	A	903	A1H1Z	C46-C40-N13	-3.35	116.85	123.46
3	A	903	A1H1Z	O04-C17-N04	-3.13	116.89	123.03
3	A	903	A1H1Z	C47-C46-C40	2.93	121.65	117.61
2	A	901	BOG	C1'-O1-C1	2.89	118.62	113.68
3	A	903	A1H1Z	C39-C38-N10	2.84	121.83	115.64
3	A	903	A1H1Z	C07-C06-C05	2.78	121.70	111.89
3	A	903	A1H1Z	O05-C23-C26	-2.77	111.15	122.03
3	A	903	A1H1Z	C29-N09-N08	-2.72	108.11	110.75
3	A	903	A1H1Z	C30-N09-C29	-2.67	123.85	128.83
3	A	903	A1H1Z	N12-C41-N11	2.59	121.78	116.18
2	A	901	BOG	C1-O5-C5	2.52	118.65	113.72
3	A	903	A1H1Z	C38-C39-N11	-2.52	105.08	112.43
3	A	903	A1H1Z	O08-N01-C04	2.49	119.59	113.76
2	A	902	BOG	O1-C1-C2	2.41	111.93	108.27
3	A	903	A1H1Z	O14-C38-N10	-2.36	118.41	123.03
3	A	903	A1H1Z	O01-C25-O02	-2.31	119.84	124.26
3	A	903	A1H1Z	C37-N10-C38	2.21	126.93	122.82
3	A	903	A1H1Z	C48-C47-C46	-2.10	117.65	120.24
3	A	903	A1H1Z	C18-N04-C17	2.01	126.56	122.82
2	A	901	BOG	O5-C1-O1	-2.01	105.31	110.04

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	BOG	O5-C1-O1-C1'
2	A	902	BOG	C2'-C1'-O1-C1
3	A	903	A1H1Z	C11-C12-C13-N03
3	A	903	A1H1Z	C12-C13-N03-C14
3	A	903	A1H1Z	C12-C13-N03-O09
3	A	903	A1H1Z	C14-C15-C16-C17
3	A	903	A1H1Z	C03-C04-N01-C05
3	A	903	A1H1Z	C03-C04-N01-O08
3	A	903	A1H1Z	N01-C05-C06-C07
3	A	903	A1H1Z	C05-C06-C07-C08
4	A	904	GOL	O1-C1-C2-C3
3	A	903	A1H1Z	O02-C25-O01-C27
2	A	901	BOG	C4-C5-C6-O6
3	A	903	A1H1Z	C16-C17-N04-C18
3	A	903	A1H1Z	C07-C08-N02-C09
3	A	903	A1H1Z	N06-C25-O01-C27
2	A	901	BOG	O5-C5-C6-O6
3	A	903	A1H1Z	O04-C17-N04-C18
3	A	903	A1H1Z	O06-C08-N02-C09
3	A	903	A1H1Z	O14-C38-N10-C37
3	A	903	A1H1Z	O13-C36-C37-N10
3	A	903	A1H1Z	N02-C09-C10-C11
3	A	903	A1H1Z	C18-C19-C20-C21
2	A	901	BOG	C2-C1-O1-C1'
3	A	903	A1H1Z	C39-C38-N10-C37
4	A	904	GOL	O1-C1-C2-O2
2	A	901	BOG	C2'-C3'-C4'-C5'
3	A	903	A1H1Z	O03-C05-C06-C07
2	A	902	BOG	C1'-C2'-C3'-C4'
2	A	902	BOG	C2'-C3'-C4'-C5'
3	A	903	A1H1Z	C24-C01-C02-C03
3	A	903	A1H1Z	C38-C39-N11-C40
3	A	903	A1H1Z	C09-C10-C11-C12
2	A	901	BOG	C1'-C2'-C3'-C4'
3	A	903	A1H1Z	C02-C03-C04-N01
2	A	901	BOG	C4'-C5'-C6'-C7'
2	A	901	BOG	C2'-C1'-O1-C1
3	A	903	A1H1Z	O01-C25-N06-C24
3	A	903	A1H1Z	O14-C38-C39-N11
3	A	903	A1H1Z	O07-C14-C15-C16
3	A	903	A1H1Z	O02-C25-N06-C24
3	A	903	A1H1Z	N03-C14-C15-C16

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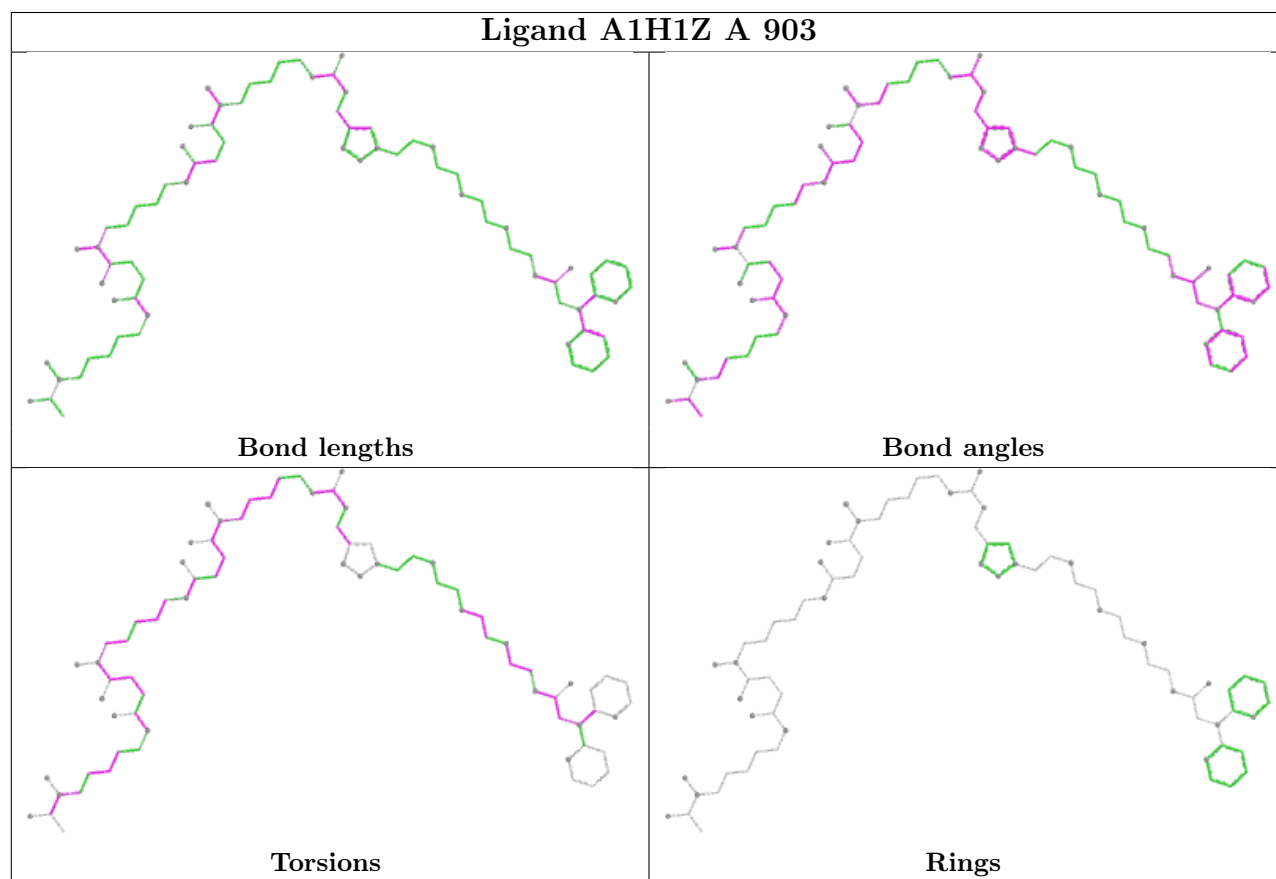
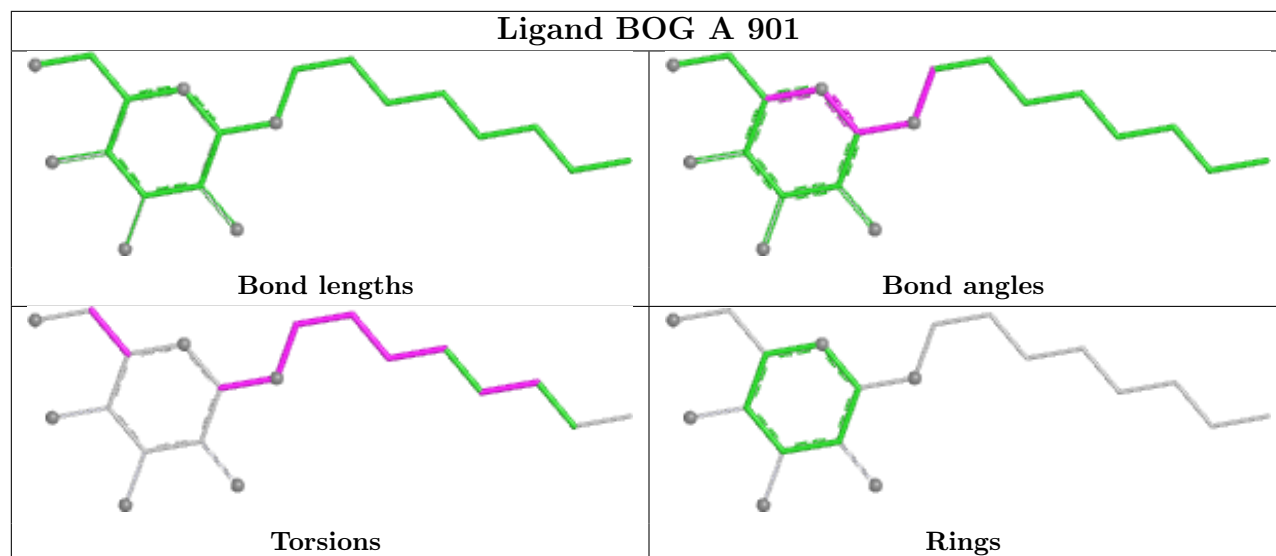
Mol	Chain	Res	Type	Atoms
3	A	903	A1H1Z	C01-C02-C03-C04
3	A	903	A1H1Z	C37-C36-O13-C35
3	A	903	A1H1Z	N10-C38-C39-N11
2	A	902	BOG	C3'-C4'-C5'-C6'
3	A	903	A1H1Z	O12-C34-C35-O13
3	A	903	A1H1Z	O01-C27-C28-C29
2	A	901	BOG	O1-C1'-C2'-C3'
3	A	903	A1H1Z	C35-C34-O12-C33
3	A	903	A1H1Z	C19-C20-C21-C22
3	A	903	A1H1Z	C26-C23-N05-O10
3	A	903	A1H1Z	O01-C27-C28-N07
3	A	903	A1H1Z	C21-C22-N05-O10
3	A	903	A1H1Z	N12-C41-N11-C39
3	A	903	A1H1Z	C45-C41-N11-C39
3	A	903	A1H1Z	O05-C23-N05-O10
3	A	903	A1H1Z	O03-C05-N01-O08
3	A	903	A1H1Z	O07-C14-N03-O09

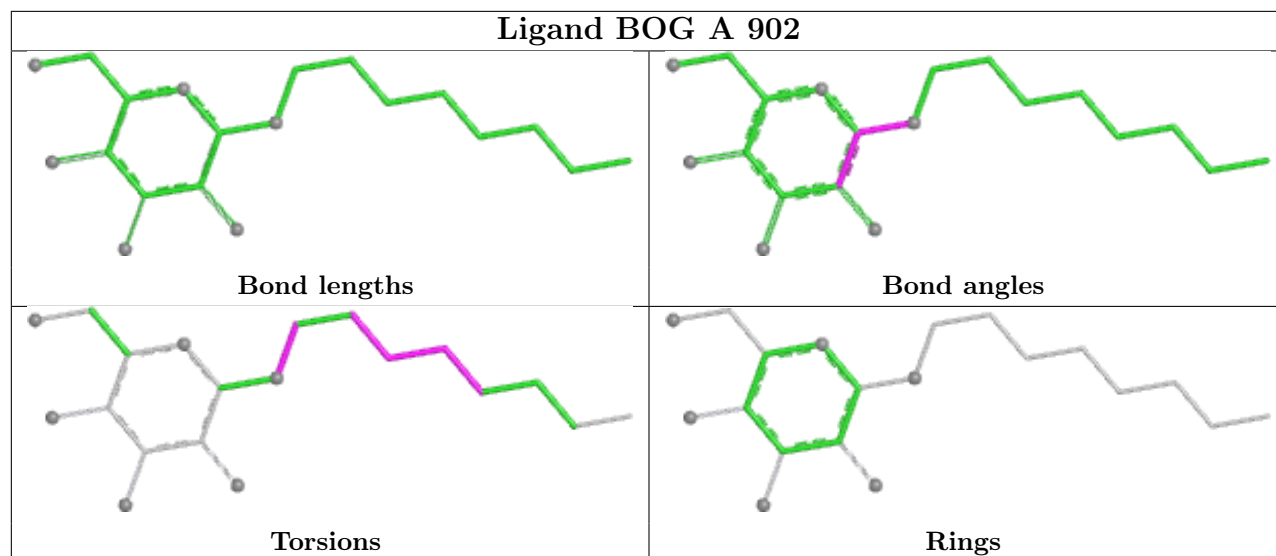
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	903	A1H1Z	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 ⓘ

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, 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	677/820 (82%)	1.01	103 (15%) 5 4	38, 82, 147, 234	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	445	TYR	5.4
1	A	223	GLY	5.1
1	A	775	LEU	5.0
1	A	412	PHE	5.0
1	A	733	LEU	4.8
1	A	400	PRO	4.5
1	A	752	LYS	4.5
1	A	730	ALA	4.5
1	A	756	LEU	4.4
1	A	275	PRO	4.4
1	A	353	PHE	4.4
1	A	224	PHE	4.2
1	A	663	PHE	4.2
1	A	780	LEU	4.1
1	A	650	THR	4.1
1	A	614	ALA	3.9
1	A	806	PHE	3.9
1	A	801	LEU	3.9
1	A	755	THR	3.9
1	A	714	GLN	3.7
1	A	732	PRO	3.7
1	A	753	GLU	3.6
1	A	777	LEU	3.6
1	A	789	LEU	3.6
1	A	421	ASP	3.6
1	A	144	VAL	3.5
1	A	298	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	396	PHE	3.5
1	A	772	LEU	3.4
1	A	784	LEU	3.4
1	A	820	PHE	3.4
1	A	399	GLU	3.4
1	A	424	TRP	3.3
1	A	736	LEU	3.3
1	A	745	VAL	3.3
1	A	398	GLY	3.3
1	A	206	PHE	3.3
1	A	795	VAL	3.2
1	A	391	ILE	3.2
1	A	738	ILE	3.2
1	A	404	ASP	3.2
1	A	403	ASP	3.2
1	A	713	ASN	3.1
1	A	456	ASN	3.1
1	A	689	LEU	3.1
1	A	401	SER	3.1
1	A	455	LEU	3.0
1	A	759	PRO	3.0
1	A	683	LEU	3.0
1	A	519	GLY	3.0
1	A	754	ASN	3.0
1	A	629	LEU	2.9
1	A	479	PHE	2.9
1	A	294	ILE	2.9
1	A	700	TYR	2.9
1	A	802	ASP	2.9
1	A	304	LYS	2.8
1	A	731	GLY	2.8
1	A	469	TYR	2.8
1	A	799	TYR	2.8
1	A	728	PHE	2.8
1	A	761	TYR	2.7
1	A	383	LEU	2.7
1	A	483	ALA	2.7
1	A	764	VAL	2.7
1	A	200	ARG	2.7
1	A	782	VAL	2.7
1	A	790	LEU	2.6
1	A	542	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	712	PRO	2.5
1	A	183	THR	2.5
1	A	748	THR	2.5
1	A	420	ILE	2.5
1	A	447	TRP	2.5
1	A	209	GLN	2.5
1	A	774	LYS	2.4
1	A	522	ALA	2.4
1	A	392	SER	2.4
1	A	220	VAL	2.4
1	A	145	PHE	2.3
1	A	274	LEU	2.3
1	A	687	LEU	2.3
1	A	458	TYR	2.3
1	A	523	ILE	2.2
1	A	763	LEU	2.2
1	A	582	PHE	2.2
1	A	803	PHE	2.2
1	A	525	TYR	2.2
1	A	314	LEU	2.2
1	A	442	VAL	2.2
1	A	706	GLY	2.2
1	A	768	ILE	2.2
1	A	505	SER	2.2
1	A	517	VAL	2.2
1	A	513	ALA	2.2
1	A	792	LYS	2.2
1	A	361	LEU	2.1
1	A	625	LYS	2.1
1	A	444	ALA	2.0
1	A	496	ARG	2.0
1	A	594	ASN	2.0
1	A	770	TYR	2.0
1	A	602	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

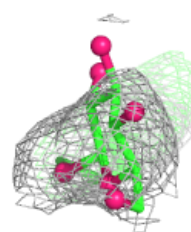
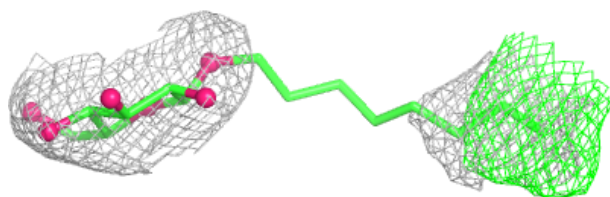
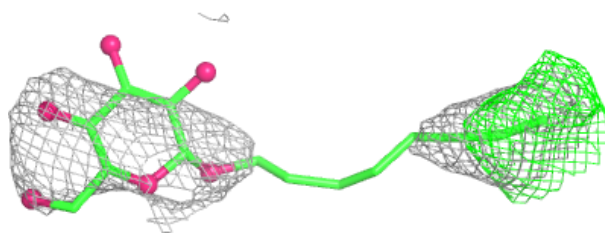
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BOG	A	901	20/20	0.45	0.24	124,155,172,178	0
7	SO4	A	909	5/5	0.57	0.15	94,112,134,151	0
7	SO4	A	908	5/5	0.66	0.11	116,125,129,134	0
7	SO4	A	910	5/5	0.77	0.10	67,85,97,102	0
8	NA	A	913	1/1	0.79	0.09	55,55,55,55	0
2	BOG	A	902	20/20	0.82	0.19	87,144,165,182	0
7	SO4	A	912	5/5	0.83	0.16	83,101,107,134	0
7	SO4	A	907	5/5	0.85	0.11	77,77,90,99	0
4	GOL	A	904	6/6	0.85	0.14	76,87,89,91	0
3	A1H1Z	A	903	76/76	0.87	0.19	51,112,187,222	0
7	SO4	A	911	5/5	0.89	0.14	113,114,135,138	0
5	NH4	A	905	1/1	0.93	0.17	56,56,56,56	0
6	FE	A	906	1/1	1.00	0.04	50,50,50,50	0

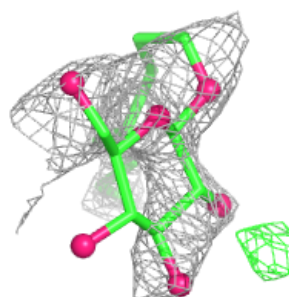
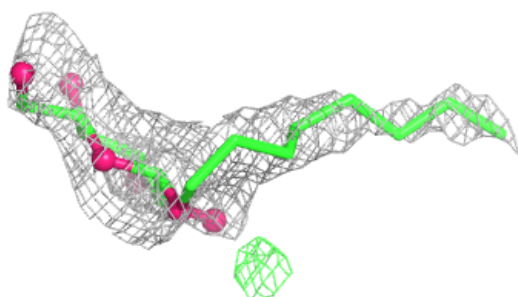
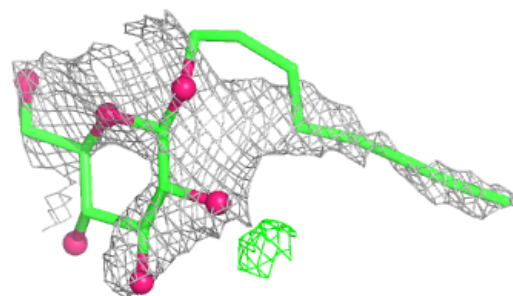
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BOG A 901:

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

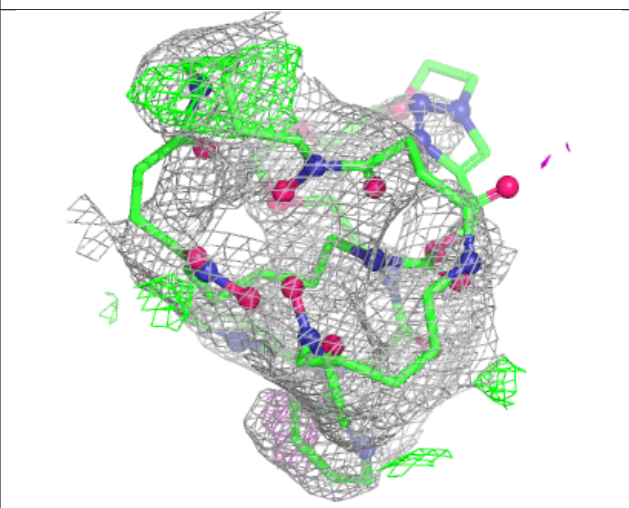
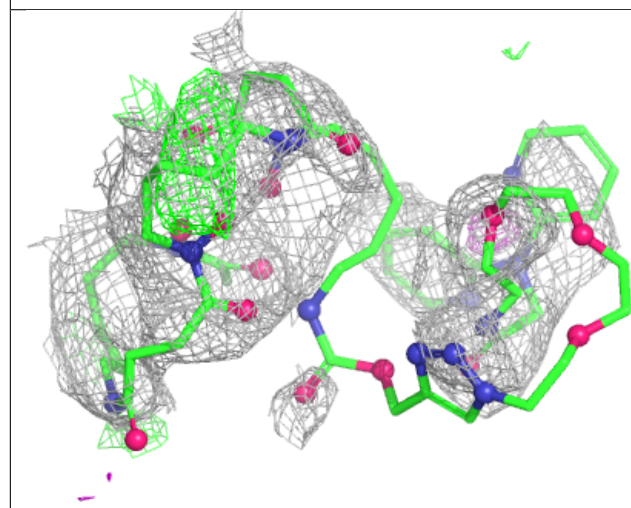
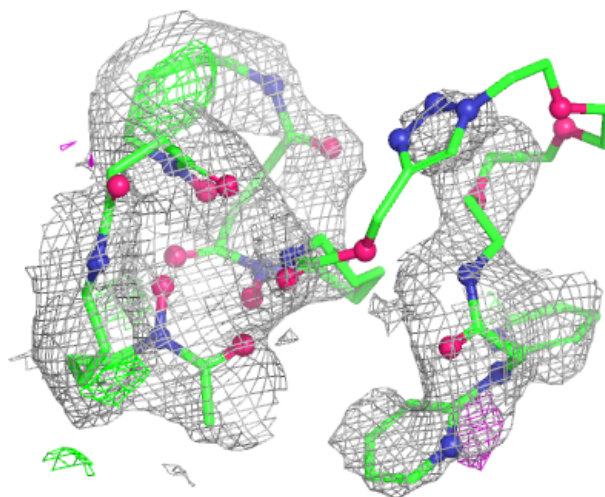
**Electron density around BOG A 902:**

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



Electron density around A1H1Z A 903:

$2mF_o-DF_c$ (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.