



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:13 PM UTC

PDB ID : 7OP6 / pdb_00007op6
Title : Bacteroides thetaiotaomicron mannosidase GH2 with beta-manno-configured cyclophellitol aziridine
Authors : McGregor, N.G.S.; Beenakker, T.J.M.; Kuo, C.; Wong, C.; Offen, W.A.; Armstrong, Z.; Codee, J.D.C.; Aerts, J.M.F.G.; Florea, B.I.; Overkleeft, H.S.; Davies, G.J.
Deposited on : 2021-05-29
Resolution : 2.05 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](#) ①) 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

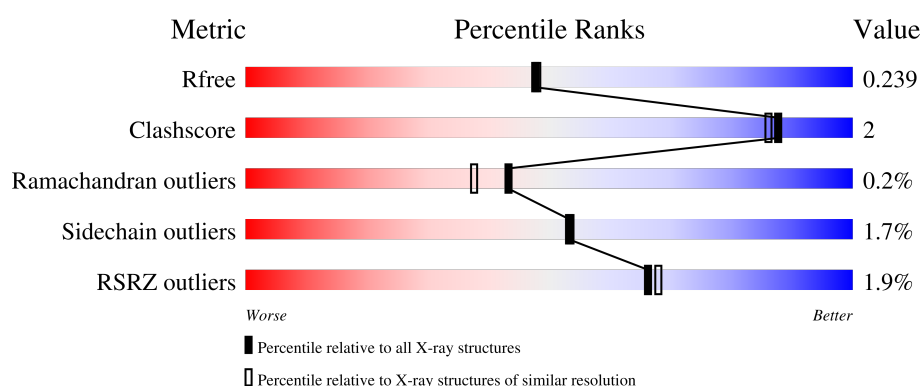
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	849	
1	B	849	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14789 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 Beta-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	837	Total	C	N	O	S	0	11	0
			6810	4367	1140	1271	32			
1	B	839	Total	C	N	O	S	0	18	0
			6878	4416	1152	1275	35			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	initiating methionine	UNP Q8AAK6
A	25	GLY	-	expression tag	UNP Q8AAK6
A	865	LEU	-	expression tag	UNP Q8AAK6
A	866	GLU	-	expression tag	UNP Q8AAK6
A	867	HIS	-	expression tag	UNP Q8AAK6
A	868	HIS	-	expression tag	UNP Q8AAK6
A	869	HIS	-	expression tag	UNP Q8AAK6
A	870	HIS	-	expression tag	UNP Q8AAK6
A	871	HIS	-	expression tag	UNP Q8AAK6
A	872	HIS	-	expression tag	UNP Q8AAK6
B	24	MET	-	initiating methionine	UNP Q8AAK6
B	25	GLY	-	expression tag	UNP Q8AAK6
B	865	LEU	-	expression tag	UNP Q8AAK6
B	866	GLU	-	expression tag	UNP Q8AAK6
B	867	HIS	-	expression tag	UNP Q8AAK6
B	868	HIS	-	expression tag	UNP Q8AAK6
B	869	HIS	-	expression tag	UNP Q8AAK6
B	870	HIS	-	expression tag	UNP Q8AAK6
B	871	HIS	-	expression tag	UNP Q8AAK6
B	872	HIS	-	expression tag	UNP Q8AAK6

- Molecule 2 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Br	0	0
			6	6		
2	B	4	Total	Br	0	0
			4	4		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 8	C 4	O 4	0	1
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 8	C 4	O 4	0	1
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0

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

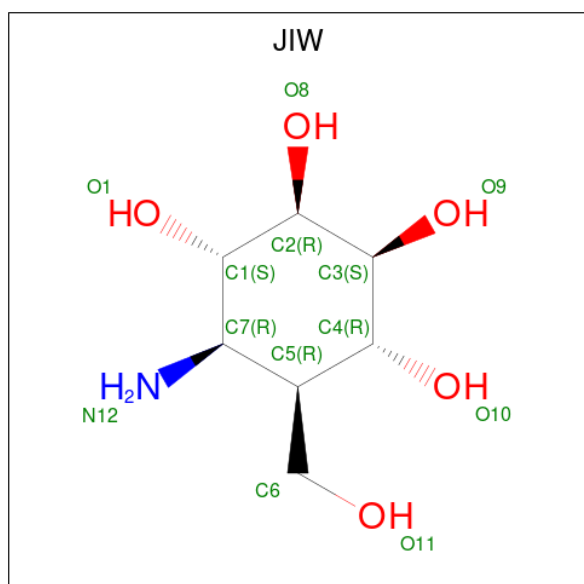
- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	6	Total	Cl		0	0
			6	6			
4	B	8	Total	Cl		0	0
			8	8			

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

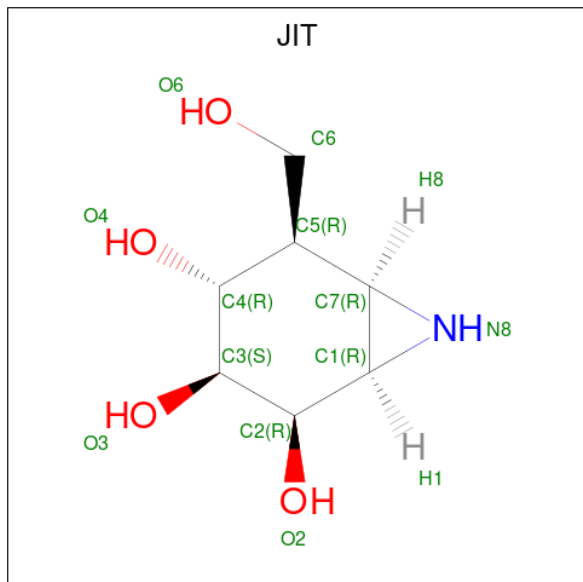
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	2	Total	Na		0	0
			2	2			
5	B	1	Total	Na		0	0
			1	1			

- Molecule 6 is beta-D-manno-configured cyclophellitol aziridine, reacted form (CCD ID: JIW) (formula: C₇H₁₅NO₅) (labeled as "Ligand of Interest" by depositor).



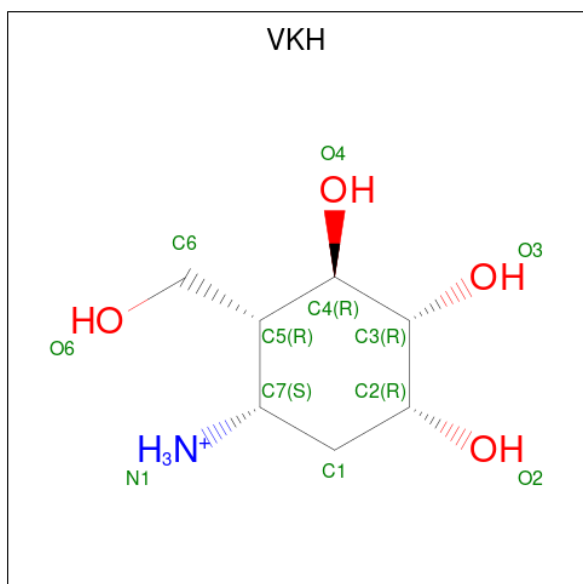
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 7 is beta-D-manno-configured cyclophellitol aziridine (CCD ID: JIT) (formula: $C_7H_{13}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	1
			12	7	1	4		

- Molecule 8 is (1 {R},2 {R},3 {S},4 {R},5 {R},6 {R})-5-(hydroxymethyl)-7-azabicyclo[4.1.0]heptane-2,3,4-triol (CCD ID: VKH) (formula: $C_7H_{16}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	1
			12	7	1	4		

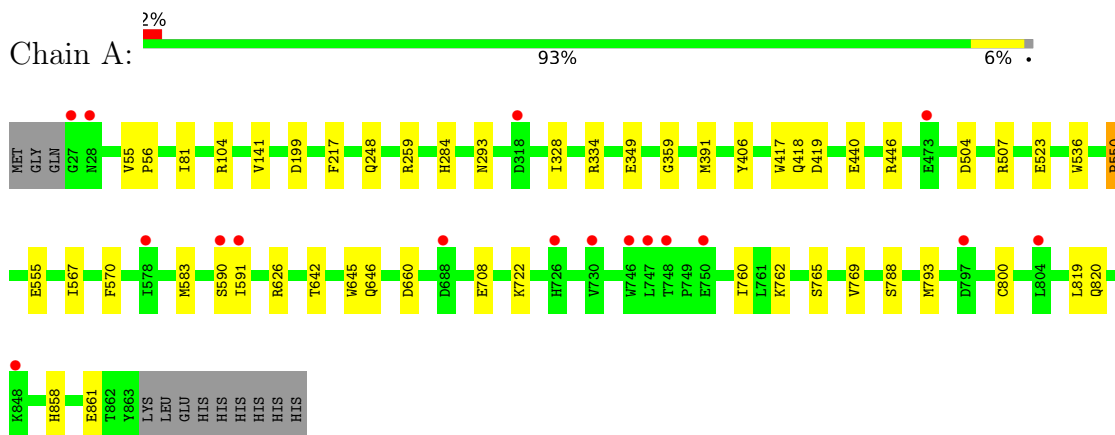
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	490	Total 492	O 492	0	2
9	B	410	Total 410	O 410	0	0

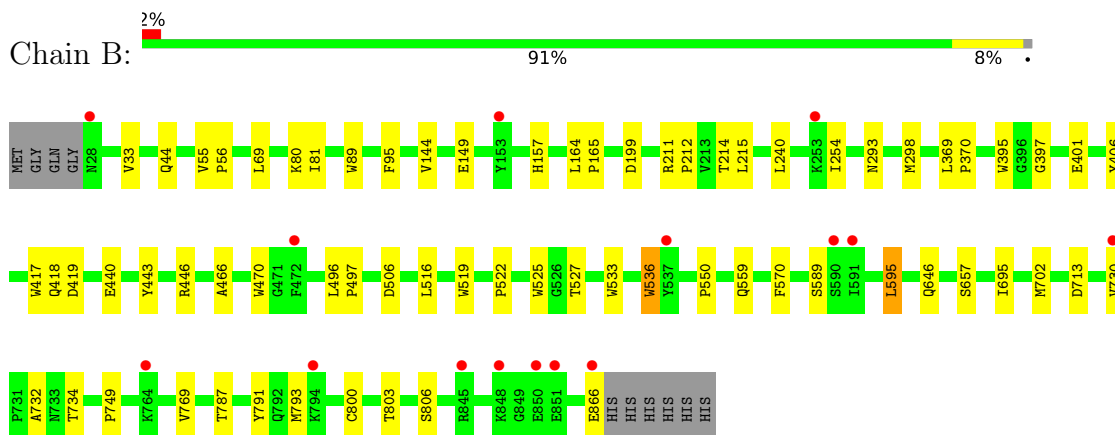
3 Residue-property plots

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: Beta-mannosidase



• Molecule 1: Beta-mannosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.92Å 116.86Å 100.84Å 90.00° 114.15° 90.00°	Depositor
Resolution (Å)	92.19 – 2.05 92.02 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.5 (92.19-2.05) 97.3 (92.02-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.185 , 0.233 0.193 , 0.239	Depositor DCC
R_{free} test set	5938 reflections (2.24%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14789	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BR, NA, JIW, VKH, EDO, JIT, CL

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	1.13	2/7020 (0.0%)	1.29	7/9550 (0.1%)
1	B	1.12	1/7095 (0.0%)	1.29	4/9649 (0.0%)
All	All	1.13	3/14115 (0.0%)	1.29	11/19199 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	555	GLU	CD-OE2	11.80	1.47	1.25
1	B	254	ILE	N-CA	5.55	1.50	1.45
1	A	293	ASN	N-CA	5.32	1.50	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	419	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	523	GLU	CB-CG-CD	5.58	122.08	112.60
1	B	713	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	550	PRO	N-CA-CB	-5.44	97.54	103.25
1	B	293	ASN	CB-CA-C	5.40	115.70	111.00
1	A	660	ASP	CA-CB-CG	5.36	117.95	112.60
1	B	570	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	141	VAL	CA-C-O	-5.26	115.36	119.46
1	A	642	THR	CB-CA-C	5.08	117.66	110.24
1	A	199	ASP	CA-CB-CG	5.05	117.65	112.60

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	6810	0	6505	18	0
1	B	6878	0	6583	34	0
2	A	6	0	0	0	0
2	B	4	0	0	0	0
3	A	60	0	90	4	0
3	B	76	0	114	5	0
4	A	6	0	0	0	0
4	B	8	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	12	0	0	1	0
7	B	12	0	0	1	0
8	B	12	0	0	0	0
9	A	492	0	0	0	0
9	B	410	0	0	1	0
All	All	14789	0	13292	53	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 2.

All (53) 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:B:793:MET:SD	1:B:800[B]:CYS:SG	2.75	0.83
1:B:519:TRP:CD1	1:B:533[B]:TRP:HB2	2.16	0.81
1:B:695:ILE:HG23	3:B:916:EDO:H22	1.65	0.78
1:B:406[A]:TYR:OH	1:B:418:GLN:OE1	2.14	0.64
6:A:930:JIW:N12	6:A:930:JIW:O11	2.30	0.64
1:A:406[B]:TYR:OH	1:A:418:GLN:OE1	2.14	0.61
1:B:69:LEU:HD22	1:B:81:ILE:HG22	1.84	0.59
1:B:536:TRP:CH2	1:B:559:GLN:HB2	2.43	0.54
1:B:33:VAL:HG13	1:B:214:THR:HG23	1.90	0.54
1:B:793:MET:CG	1:B:800[B]:CYS:SG	2.96	0.54
1:B:443:TYR:HA	3:B:922:EDO:H12	1.90	0.53
1:A:284:HIS:CE1	3:A:920:EDO:O1	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:NH1	3:A:919:EDO:O1	2.43	0.52
1:B:33:VAL:HG13	1:B:214:THR:CG2	2.42	0.50
1:A:55:VAL:HA	1:A:56:PRO:C	2.36	0.50
1:B:516:LEU:HD23	1:B:527:THR:HG21	1.94	0.48
1:A:793:MET:SD	1:A:800[A]:CYS:SG	3.10	0.48
1:A:359:GLY:HA3	1:A:391:MET:O	2.14	0.47
1:A:328:ILE:HG23	3:A:908:EDO:H12	1.95	0.47
1:B:199:ASP:OD2	7:B:901[A]:JIT:O6	2.31	0.47
1:A:504:ASP:OD2	1:A:507:ARG:HD2	2.14	0.47
1:B:164:LEU:N	1:B:165:PRO:HD2	2.29	0.47
1:A:446:ARG:HD3	3:A:919:EDO:O1	2.15	0.47
1:A:567:ILE:HA	1:A:570:PHE:CE2	2.51	0.45
1:A:858:HIS:CE1	1:A:861:GLU:HG3	2.52	0.45
1:B:695:ILE:CG2	3:B:916:EDO:H22	2.42	0.45
1:B:401:GLU:O	1:B:406[B]:TYR:HE1	2.00	0.45
1:A:567:ILE:HG23	1:A:583:MET:HE1	1.98	0.44
1:B:395:TRP:CH2	1:B:397:GLY:HA3	2.53	0.44
1:B:522:PRO:HA	1:B:525:TRP:CE2	2.52	0.44
1:B:55:VAL:HA	1:B:56:PRO:C	2.42	0.44
1:B:791:TYR:HA	1:B:803:THR:O	2.16	0.44
1:A:334:ARG:NH1	1:A:349[B]:GLU:OE1	2.51	0.44
1:B:496:LEU:N	1:B:497:PRO:HD2	2.33	0.43
1:B:446:ARG:HH11	3:B:922:EDO:H11	1.85	0.42
1:A:793:MET:HG3	1:A:800[A]:CYS:SG	2.60	0.42
1:B:157:HIS:CE1	3:B:919:EDO:H12	2.54	0.42
1:A:708:GLU:OE1	1:A:762:LYS:NZ	2.40	0.42
1:B:702:MET:HB2	1:B:730:VAL:HB	2.00	0.42
1:A:645:TRP:HA	1:A:646:GLN:HA	1.87	0.42
1:B:369:LEU:N	1:B:370:PRO:CD	2.82	0.41
1:B:646:GLN:O	1:B:657:SER:HA	2.21	0.41
1:A:104:ARG:HG3	1:A:217:PHE:HB3	2.03	0.41
1:B:95:PHE:CE2	1:B:215:LEU:HD11	2.55	0.41
1:B:211:ARG:HB3	1:B:212:PRO:CD	2.51	0.41
1:B:595:LEU:HD12	1:B:595:LEU:HA	1.83	0.41
1:A:820:GLN:HA	1:A:820:GLN:OE1	2.21	0.41
1:B:787:THR:OG1	1:B:806[A]:SER:OG	2.38	0.41
1:B:732:ALA:O	1:B:734:THR:HG23	2.21	0.40
1:B:466:ALA:HA	1:B:470:TRP:CG	2.57	0.40
1:B:44:GLN:HB2	1:B:89:TRP:CZ3	2.57	0.40
1:B:298:MET:HE3	1:B:298:MET:HA	2.04	0.40
1:B:506:ASP:HB2	9:B:1014:HOH:O	2.21	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	846/849 (100%)	821 (97%)	22 (3%)	3 (0%)	30	22
1	B	855/849 (101%)	830 (97%)	24 (3%)	1 (0%)	48	43
All	All	1701/1698 (100%)	1651 (97%)	46 (3%)	4 (0%)	43	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	536	TRP
1	B	536	TRP
1	A	590	SER
1	A	591	ILE

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	732/756 (97%)	718 (98%)	14 (2%)	50	50
1	B	738/756 (98%)	726 (98%)	12 (2%)	55	56
All	All	1470/1512 (97%)	1444 (98%)	26 (2%)	53	51

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ILE
1	A	248	GLN
1	A	259	ARG
1	A	417	TRP
1	A	440	GLU
1	A	550	PRO
1	A	626[A]	ARG
1	A	626[B]	ARG
1	A	722	LYS
1	A	760	ILE
1	A	765	SER
1	A	769	VAL
1	A	788	SER
1	A	819	LEU
1	B	80	LYS
1	B	144	VAL
1	B	149	GLU
1	B	240	LEU
1	B	417	TRP
1	B	440	GLU
1	B	550	PRO
1	B	589	SER
1	B	595	LEU
1	B	749	PRO
1	B	769	VAL
1	B	866	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	86	ASN
1	A	162	GLN
1	A	178	ASN
1	A	230	GLN
1	A	237	ASN
1	A	623	GLN
1	A	767	HIS
1	A	783	GLN
1	B	313	GLN
1	B	388	ASN
1	B	733	ASN
1	B	768	GLN

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 64 ligands modelled in this entry, 27 are monoatomic - leaving 37 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	B	922	-	3,3,3	0.06	0	2,2,2	0.23	0
3	EDO	A	915	-	3,3,3	0.18	0	2,2,2	0.23	0
6	JIW	A	930	1	12,12,13	0.99	0	14,17,19	1.24	2 (14%)
3	EDO	B	908	-	3,3,3	0.05	0	2,2,2	0.08	0
3	EDO	B	916	-	3,3,3	0.35	0	2,2,2	0.81	0
3	EDO	A	920	-	3,3,3	0.28	0	2,2,2	0.18	0
3	EDO	A	911	-	3,3,3	0.17	0	2,2,2	0.08	0
3	EDO	A	921	-	3,3,3	0.17	0	2,2,2	0.04	0
7	JIT	B	901[A]	-	13,13,13	1.79	2 (15%)	15,20,20	1.51	3 (20%)
3	EDO	A	907	-	3,3,3	0.19	0	2,2,2	0.21	0
3	EDO	A	909	-	3,3,3	0.20	0	2,2,2	0.24	0
3	EDO	A	917	-	3,3,3	0.09	0	2,2,2	0.09	0
3	EDO	B	909	-	3,3,3	0.25	0	2,2,2	0.39	0
3	EDO	A	910	-	3,3,3	0.04	0	2,2,2	0.06	0
3	EDO	B	914	-	3,3,3	0.04	0	2,2,2	0.04	0
3	EDO	A	908	-	3,3,3	0.17	0	2,2,2	0.33	0
3	EDO	B	915	-	3,3,3	0.41	0	2,2,2	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	913[A]	-	3,3,3	0.12	0	2,2,2	0.05	0
3	EDO	A	913	-	3,3,3	0.08	0	2,2,2	0.04	0
3	EDO	A	919	-	3,3,3	0.10	0	2,2,2	0.17	0
3	EDO	A	912	-	3,3,3	0.19	0	2,2,2	0.09	0
3	EDO	B	907[B]	-	3,3,3	0.11	0	2,2,2	0.04	0
3	EDO	B	919	-	3,3,3	0.47	0	2,2,2	0.20	0
3	EDO	A	918	-	3,3,3	0.05	0	2,2,2	0.21	0
3	EDO	B	920	-	3,3,3	0.11	0	2,2,2	0.11	0
3	EDO	B	917	-	3,3,3	0.18	0	2,2,2	0.15	0
3	EDO	B	911	-	3,3,3	0.28	0	2,2,2	0.57	0
3	EDO	B	906	-	3,3,3	0.15	0	2,2,2	0.39	0
3	EDO	B	918	-	3,3,3	0.24	0	2,2,2	0.15	0
3	EDO	A	914	-	3,3,3	0.34	0	2,2,2	0.54	0
8	VKH	B	932[B]	1	12,12,12	0.83	0	14,17,17	1.34	2 (14%)
3	EDO	B	921	-	3,3,3	0.57	0	2,2,2	0.47	0
3	EDO	B	912	-	3,3,3	0.05	0	2,2,2	0.10	0
3	EDO	B	913[B]	-	3,3,3	0.14	0	2,2,2	0.30	0
3	EDO	A	916	-	3,3,3	0.13	0	2,2,2	0.13	0
3	EDO	B	907[A]	-	3,3,3	0.11	0	2,2,2	0.09	0
3	EDO	B	910	-	3,3,3	0.14	0	2,2,2	0.27	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	B	922	-	-	1/1/1/1	-
3	EDO	A	915	-	-	1/1/1/1	-
6	JIW	A	930	1	-	1/2/22/26	0/1/1/1
3	EDO	B	908	-	-	0/1/1/1	-
3	EDO	B	916	-	-	0/1/1/1	-
3	EDO	A	920	-	-	0/1/1/1	-
3	EDO	A	911	-	-	1/1/1/1	-
3	EDO	A	921	-	-	1/1/1/1	-
7	JIT	B	901[A]	-	-	1/2/27/27	0/2/2/2
3	EDO	A	907	-	-	0/1/1/1	-
3	EDO	A	909	-	-	1/1/1/1	-
3	EDO	A	917	-	-	1/1/1/1	-
3	EDO	B	909	-	-	0/1/1/1	-
3	EDO	A	910	-	-	0/1/1/1	-
3	EDO	B	914	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	908	-	-	0/1/1/1	-
3	EDO	B	915	-	-	1/1/1/1	-
3	EDO	B	913[A]	-	-	0/1/1/1	-
3	EDO	A	913	-	-	0/1/1/1	-
3	EDO	A	919	-	-	1/1/1/1	-
3	EDO	A	912	-	-	0/1/1/1	-
3	EDO	B	907[B]	-	-	0/1/1/1	-
3	EDO	B	919	-	-	1/1/1/1	-
3	EDO	A	918	-	-	0/1/1/1	-
3	EDO	B	920	-	-	1/1/1/1	-
3	EDO	B	917	-	-	0/1/1/1	-
3	EDO	B	911	-	-	1/1/1/1	-
3	EDO	B	906	-	-	0/1/1/1	-
3	EDO	B	918	-	-	0/1/1/1	-
3	EDO	A	914	-	-	1/1/1/1	-
8	VKH	B	932[B]	1	-	0/2/22/22	0/1/1/1
3	EDO	B	921	-	-	0/1/1/1	-
3	EDO	B	912	-	-	1/1/1/1	-
3	EDO	B	913[B]	-	-	1/1/1/1	-
3	EDO	A	916	-	-	1/1/1/1	-
3	EDO	B	907[A]	-	-	1/1/1/1	-
3	EDO	B	910	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	901[A]	JIT	C7-C1	4.82	1.53	1.48
7	B	901[A]	JIT	C7-N8	2.59	1.49	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	901[A]	JIT	C7-N8-C1	3.66	61.75	60.38
8	B	932[B]	VKH	C1-C2-C3	3.32	115.45	110.67
7	B	901[A]	JIT	C1-C7-N8	-2.78	58.85	59.81
6	A	930	JIW	C1-C7-C5	2.47	114.78	111.67
6	A	930	JIW	C5-C4-C3	2.32	114.68	110.77
8	B	932[B]	VKH	C5-C7-N1	-2.26	107.17	111.73
7	B	901[A]	JIT	C3-C2-C1	2.01	113.32	110.40

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	919	EDO	O1-C1-C2-O2
3	B	922	EDO	O1-C1-C2-O2
3	A	909	EDO	O1-C1-C2-O2
3	A	921	EDO	O1-C1-C2-O2
3	B	907[A]	EDO	O1-C1-C2-O2
3	A	917	EDO	O1-C1-C2-O2
3	A	919	EDO	O1-C1-C2-O2
3	A	911	EDO	O1-C1-C2-O2
7	B	901[A]	JIT	C4-C5-C6-O6
3	B	913[B]	EDO	O1-C1-C2-O2
3	B	915	EDO	O1-C1-C2-O2
3	B	920	EDO	O1-C1-C2-O2
3	A	914	EDO	O1-C1-C2-O2
3	A	916	EDO	O1-C1-C2-O2
3	B	910	EDO	O1-C1-C2-O2
3	A	915	EDO	O1-C1-C2-O2
3	B	912	EDO	O1-C1-C2-O2
3	B	911	EDO	O1-C1-C2-O2
3	B	914	EDO	O1-C1-C2-O2
6	A	930	JIW	C7-C5-C6-O11

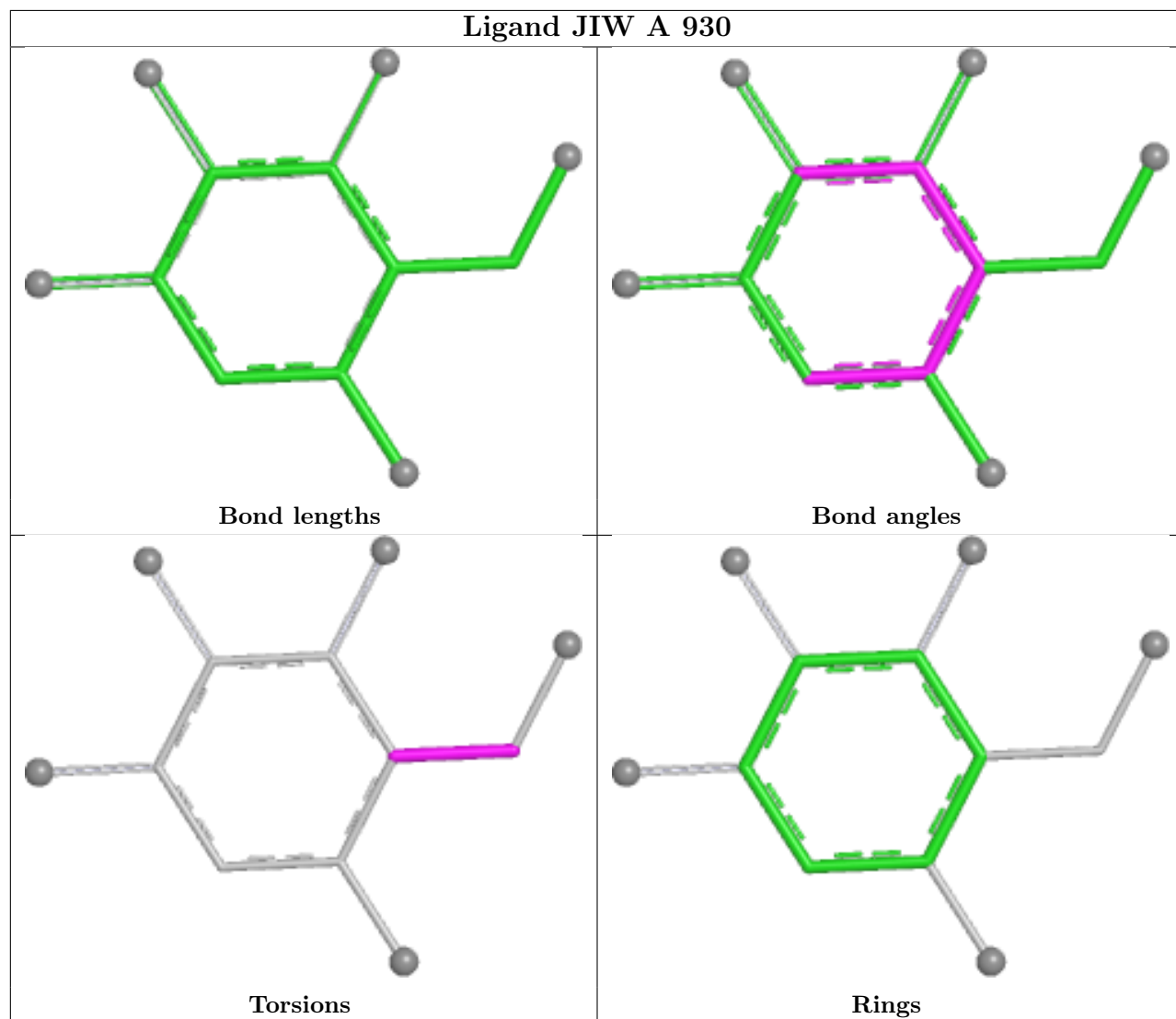
There are no ring outliers.

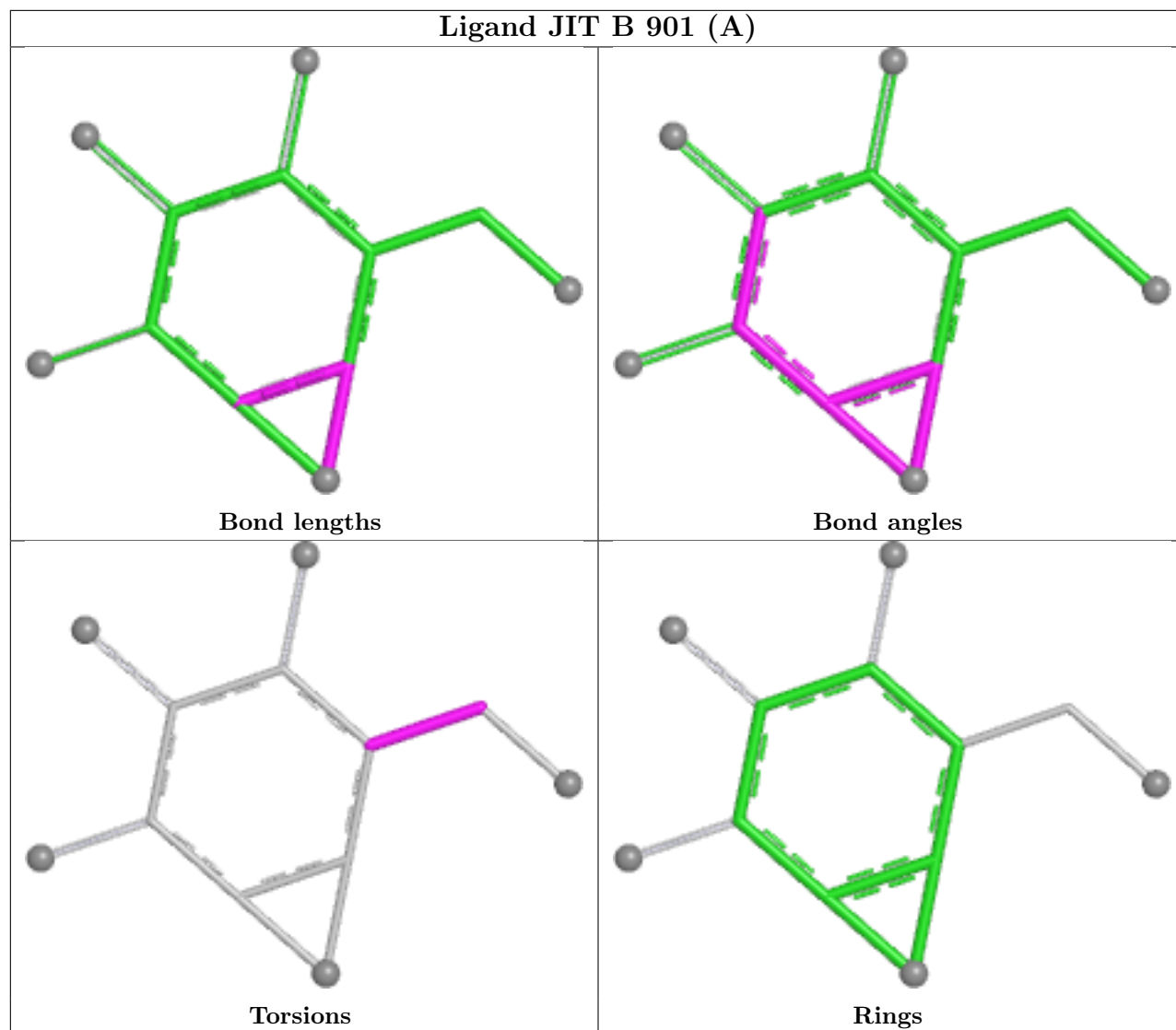
8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	922	EDO	2	0
6	A	930	JIW	1	0
3	B	916	EDO	2	0
3	A	920	EDO	1	0
7	B	901[A]	JIT	1	0
3	A	908	EDO	1	0
3	A	919	EDO	2	0
3	B	919	EDO	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	837/849 (98%)	0.03	17 (2%) 65 67	10, 33, 54, 78	41 (4%)
1	B	839/849 (98%)	0.10	15 (1%) 67 69	11, 35, 54, 70	42 (5%)
All	All	1676/1698 (98%)	0.07	32 (1%) 66 68	10, 34, 54, 78	83 (4%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	746	TRP	6.4
1	B	28	ASN	5.8
1	A	27	GLY	4.7
1	B	472	PHE	4.7
1	B	590	SER	4.6
1	B	866	GLU	4.5
1	A	590	SER	4.3
1	A	28	ASN	4.2
1	B	850	GLU	4.2
1	A	797	ASP	4.0
1	A	591	ILE	3.8
1	A	473	GLU	3.5
1	A	578	ILE	3.4
1	B	537	TYR	3.4
1	B	851	GLU	3.3
1	B	848	LYS	3.0
1	B	591	ILE	2.8
1	A	318	ASP	2.8
1	A	747	LEU	2.7
1	A	688	ASP	2.4
1	A	848	LYS	2.3
1	B	253	LYS	2.3
1	B	730	VAL	2.3
1	B	794	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	730	VAL	2.2
1	A	726	HIS	2.1
1	B	764	LYS	2.1
1	B	153	TYR	2.1
1	A	748	THR	2.1
1	A	750	GLU	2.1
1	A	804	LEU	2.1
1	B	845[A]	ARG	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($\text{\AA}^2$)	Q<0.9
3	EDO	B	915	4/4	0.65	0.25	25,27,28,28	4
3	EDO	B	918	4/4	0.66	0.28	33,34,34,35	4
8	VKH	B	932[B]	12/12	0.67	0.16	41,45,46,47	12
3	EDO	A	920	4/4	0.68	0.19	54,55,56,57	0
3	EDO	A	921	4/4	0.73	0.18	50,53,54,54	0
3	EDO	B	920	4/4	0.74	0.26	25,26,26,27	4
3	EDO	B	908	4/4	0.76	0.26	33,33,34,35	4
3	EDO	A	917	4/4	0.81	0.22	24,26,27,28	4
3	EDO	B	917	4/4	0.82	0.17	37,42,43,46	4
3	EDO	A	919	4/4	0.82	0.15	28,28,30,35	4
3	EDO	B	911	4/4	0.83	0.18	26,26,26,27	4
7	JIT	B	901[A]	12/12	0.83	0.15	40,51,53,53	12
3	EDO	A	912	4/4	0.83	0.23	30,32,34,35	4
4	CL	B	930	1/1	0.84	0.14	77,77,77,77	0
3	EDO	B	922	4/4	0.85	0.19	28,32,34,39	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	A	927	1/1	0.86	0.14	72,72,72,72	0
3	EDO	A	916	4/4	0.86	0.27	32,32,33,35	4
3	EDO	B	916	4/4	0.86	0.14	33,33,34,35	4
4	CL	A	925	1/1	0.86	0.14	73,73,73,73	0
3	EDO	A	907	4/4	0.88	0.17	22,22,23,23	4
3	EDO	B	919	4/4	0.89	0.14	45,48,49,64	0
5	NA	A	929	1/1	0.89	0.13	47,47,47,47	0
3	EDO	A	915	4/4	0.90	0.13	43,45,45,50	0
4	CL	B	927	1/1	0.90	0.16	67,67,67,67	0
3	EDO	B	914	4/4	0.90	0.17	58,59,63,66	0
4	CL	B	928	1/1	0.91	0.14	66,66,66,66	0
3	EDO	B	909	4/4	0.91	0.12	32,42,42,49	0
2	BR	B	904	1/1	0.91	0.09	58,58,58,58	1
4	CL	B	924	1/1	0.91	0.10	67,67,67,67	0
4	CL	A	923	1/1	0.91	0.10	56,56,56,56	0
3	EDO	A	910	4/4	0.92	0.11	45,45,46,46	0
3	EDO	B	907[A]	4/4	0.92	0.10	33,35,36,37	4
5	NA	B	931	1/1	0.92	0.18	55,55,55,55	0
6	JIW	A	930	12/13	0.92	0.08	30,33,35,37	12
3	EDO	B	907[B]	4/4	0.92	0.10	40,44,45,49	4
3	EDO	A	918	4/4	0.92	0.14	27,29,29,30	4
3	EDO	B	910	4/4	0.93	0.09	38,39,39,39	4
4	CL	A	924	1/1	0.93	0.12	71,71,71,71	0
3	EDO	A	908	4/4	0.93	0.10	31,41,45,52	0
4	CL	A	926	1/1	0.93	0.11	75,75,75,75	0
3	EDO	B	913[A]	4/4	0.93	0.12	36,36,37,37	4
3	EDO	B	913[B]	4/4	0.93	0.12	41,41,42,42	4
4	CL	A	922	1/1	0.93	0.11	47,47,47,47	0
3	EDO	B	912	4/4	0.94	0.09	46,46,49,51	0
4	CL	B	923	1/1	0.94	0.14	62,62,62,62	0
3	EDO	A	914	4/4	0.94	0.08	34,39,43,45	0
4	CL	B	925	1/1	0.94	0.10	46,46,46,46	0
3	EDO	A	913	4/4	0.94	0.09	43,50,50,51	0
3	EDO	B	906	4/4	0.94	0.09	39,41,42,45	0
3	EDO	A	909	4/4	0.95	0.07	35,37,37,43	0
2	BR	A	905	1/1	0.95	0.06	34,34,34,34	0
3	EDO	B	921	4/4	0.95	0.08	30,33,37,37	0
4	CL	B	929	1/1	0.95	0.07	45,45,45,45	0
2	BR	A	902	1/1	0.95	0.09	39,39,39,39	1
2	BR	A	903	1/1	0.96	0.05	32,32,32,32	1
2	BR	A	906	1/1	0.96	0.06	54,54,54,54	1
2	BR	B	902	1/1	0.96	0.09	44,44,44,44	0

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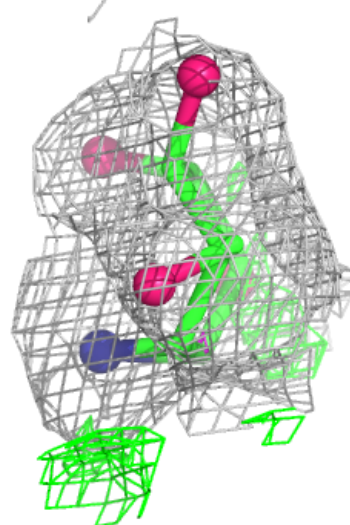
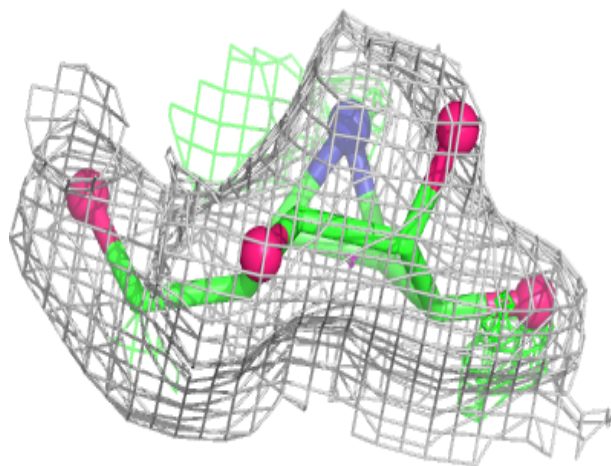
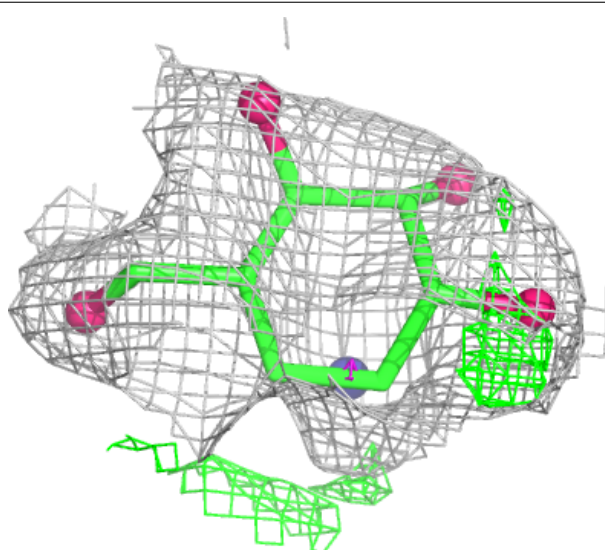
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BR	B	903	1/1	0.96	0.07	39,39,39,39	1
5	NA	A	928	1/1	0.97	0.09	33,33,33,33	0
4	CL	B	926	1/1	0.97	0.06	49,49,49,49	0
2	BR	A	904	1/1	0.97	0.04	32,32,32,32	1
3	EDO	A	911	4/4	0.97	0.06	38,39,39,39	0
2	BR	A	901	1/1	0.97	0.05	41,41,41,41	1
2	BR	B	905	1/1	0.97	0.15	41,41,41,41	1

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.

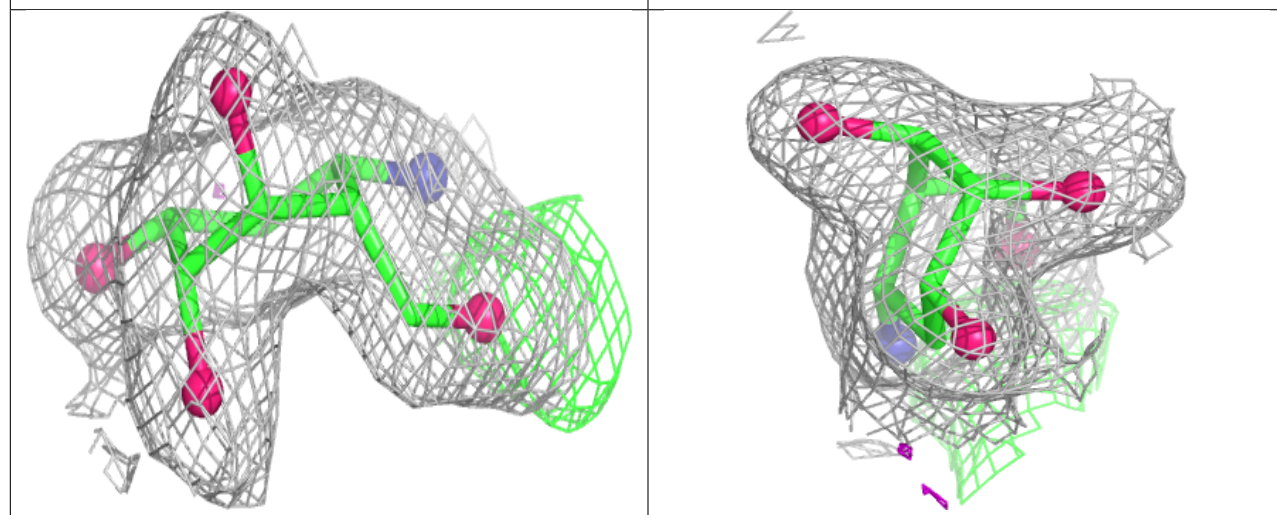
Electron density around JIT B 901 (A):

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 JIW A 930:

$2mF_o-DF_c$ (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.