



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:20 PM UTC

PDB ID : 2VUR / pdb_00002vur
Title : Chemical dissection of the link between Streptozotocin, O-GlcNAc and pancreatic cell death
Authors : Pathak, S.; Dorfmueeller, H.C.; Borodkin, V.S.; van Aalten, D.M.F.
Deposited on : 2008-05-29
Resolution : 2.20 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

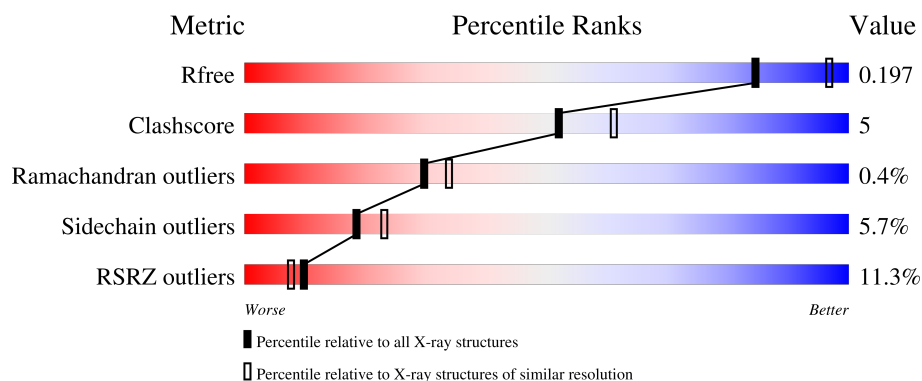
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	594	7% 83% 13% ..
1	B	594	15% 84% 12% ..

2 Entry composition [i](#)

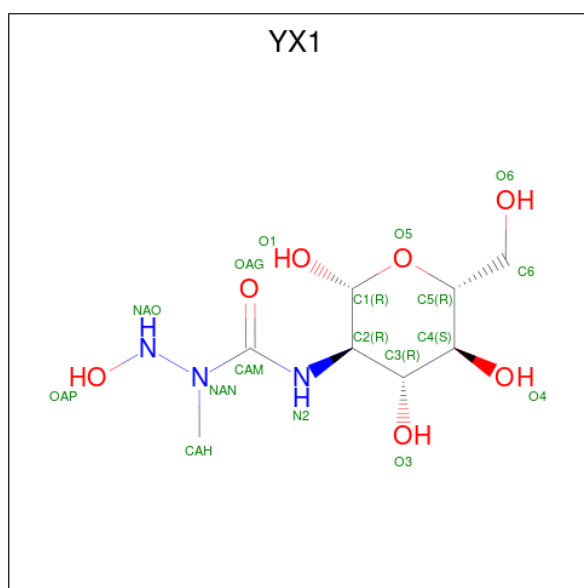
There are 4 unique types of molecules in this entry. The entry contains 9809 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 O-GLCNACASE NAGJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	0	0	0
			4620	2908	756	939	17			
1	B	584	Total	C	N	O	S	0	0	0
			4620	2908	756	939	17			

- Molecule 2 is 2-deoxy-2-[[[(2-hydroxy-1-methylhydrazino)carbonyl]amino}-beta-D-glucopyranose (CCD ID: YX1) (formula: $C_8H_{17}N_3O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	8	3	7		
2	B	1	Total	C	N	O	0	0
			18	8	3	7		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

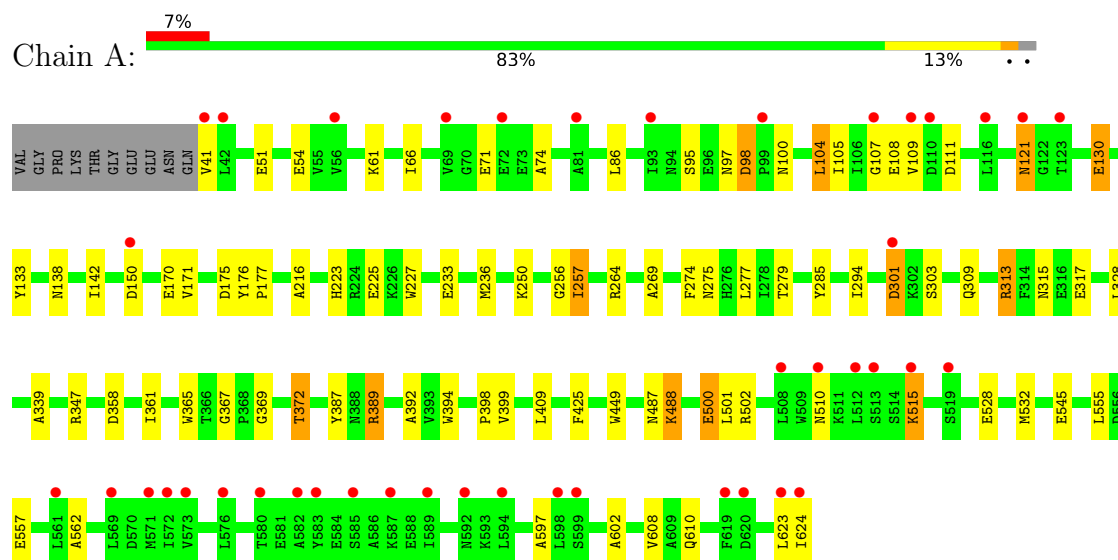
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	277	Total	O	0	0
			277	277		
4	B	251	Total	O	0	0
			251	251		

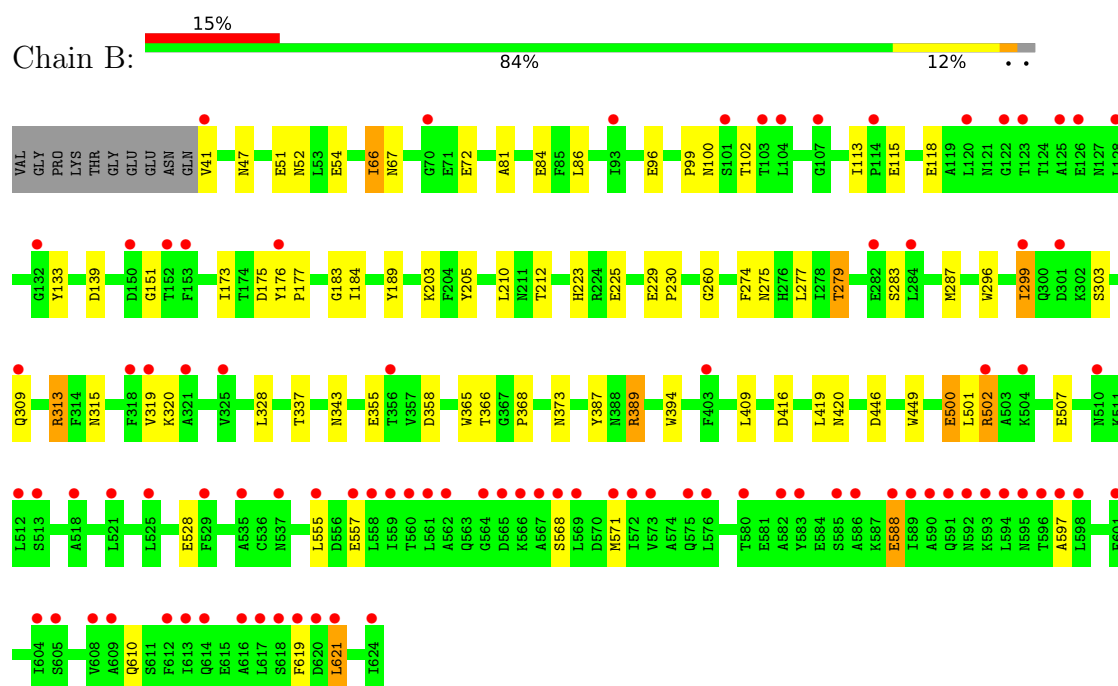
3 Residue-property plots [i](#)

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: O-GLCNACASE NAGJ



• Molecule 1: O-GLCNACASE NAGJ



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.47Å 149.73Å 152.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.20 19.91 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.91-2.20) 99.5 (19.91-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.241 0.191 , 0.197	Depositor DCC
R_{free} test set	1503 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9809	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 3.28% 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: SO4, YX1

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	0.72	0/4716	0.91	3/6403 (0.0%)
1	B	0.74	4/4716 (0.1%)	0.92	2/6403 (0.0%)
All	All	0.73	4/9432 (0.0%)	0.92	5/12806 (0.0%)

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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	ASN	CG-OD1	8.24	1.39	1.23
1	B	115	GLU	CD-OE1	7.20	1.39	1.25
1	B	67	ASN	CG-ND2	5.45	1.44	1.33
1	B	99	PRO	C-N	5.17	1.41	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ASN	OD1-CG-ND2	8.59	131.19	122.60
1	A	97	ASN	N-CA-C	6.48	119.76	110.10
1	A	367	GLY	CA-C-N	5.49	125.84	119.47
1	A	367	GLY	C-N-CA	5.49	125.84	119.47
1	B	373	ASN	N-CA-C	5.41	117.18	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4620	0	4412	49	0
1	B	4620	0	4412	43	0
2	A	18	0	17	1	0
2	B	18	0	17	2	0
3	A	5	0	0	0	0
4	A	277	0	0	3	0
4	B	251	0	0	9	0
All	All	9809	0	8858	92	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 (92) 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:502:ARG:O	1:A:502:ARG:HD3	1.62	0.98
1:B:502:ARG:O	1:B:502:ARG:HD3	1.67	0.93
1:A:389:ARG:HG2	1:A:389:ARG:HH11	1.35	0.90
1:A:227:TRP:HB2	1:A:257:ILE:HD11	1.57	0.87
1:B:296:TRP:HA	1:B:299:ILE:HD11	1.61	0.80
1:A:501:LEU:HD13	1:A:528:GLU:HG2	1.62	0.80
1:A:301:ASP:OD2	1:A:303:SER:OG	2.01	0.76
1:B:502:ARG:HD3	1:B:502:ARG:C	2.09	0.76
1:B:588:GLU:HG3	4:B:2223:HOH:O	1.86	0.74
1:A:502:ARG:HD3	1:A:502:ARG:C	2.09	0.74
1:A:557:GLU:HG3	1:A:602:ALA:HB3	1.75	0.68
1:B:274:PHE:CZ	1:B:313:ARG:HD2	2.29	0.67
1:B:387:TYR:HB3	1:B:389:ARG:HD2	1.77	0.66
1:A:108:GLU:O	1:A:111:ASP:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ARG:HG2	1:A:389:ARG:NH1	2.05	0.65
1:B:597:ALA:O	4:B:2229:HOH:O	2.15	0.64
1:B:500:GLU:HG2	4:B:2163:HOH:O	1.98	0.63
1:B:47:ASN:ND2	4:B:2004:HOH:O	2.32	0.63
1:A:285:TYR:HD2	4:A:2074:HOH:O	1.82	0.61
1:B:66:ILE:HG22	1:B:102:THR:HB	1.83	0.61
1:A:275:ASN:O	1:A:279:THR:HG23	2.01	0.60
1:B:275:ASN:O	1:B:279:THR:HG23	2.01	0.60
1:B:507:GLU:HG2	4:B:2168:HOH:O	2.01	0.60
1:A:515:LYS:HG2	1:A:624:ILE:HG22	1.82	0.60
1:B:387:TYR:O	1:B:389:ARG:HG3	2.01	0.60
1:B:274:PHE:CE2	1:B:313:ARG:HD2	2.36	0.60
1:A:313:ARG:HD3	1:A:317:GLU:OE2	2.02	0.60
1:B:47:ASN:HD21	1:B:446:ASP:HB2	1.66	0.59
1:A:274:PHE:CZ	1:A:313:ARG:HD2	2.38	0.58
1:B:501:LEU:HD13	1:B:528:GLU:HG2	1.86	0.57
1:A:610:GLN:NE2	4:A:2265:HOH:O	2.38	0.57
1:B:260:GLY:HA3	1:B:299:ILE:CD1	2.36	0.56
1:B:619:PHE:HE2	1:B:621:LEU:HG	1.71	0.55
1:B:610:GLN:NE2	4:B:2239:HOH:O	2.40	0.55
1:A:233:GLU:HA	1:A:236:MET:HG3	1.88	0.54
1:A:133:TYR:CE2	1:A:175:ASP:HB3	2.43	0.54
1:A:557:GLU:HG3	1:A:602:ALA:CB	2.38	0.53
1:B:260:GLY:HA3	1:B:299:ILE:HD13	1.91	0.52
1:A:358:ASP:O	1:A:389:ARG:NH2	2.42	0.52
1:B:315:ASN:ND2	1:B:320:LYS:HE3	2.25	0.52
1:B:337:THR:HB	1:B:368:PRO:HA	1.91	0.51
1:A:216:ALA:HB2	1:A:256:GLY:HA3	1.94	0.50
1:B:41:VAL:N	4:B:2001:HOH:O	2.44	0.50
1:A:387:TYR:O	1:A:389:ARG:HG2	2.12	0.49
1:A:500:GLU:H	1:A:500:GLU:CD	2.19	0.49
1:B:343:ASN:HB3	4:B:2078:HOH:O	2.12	0.49
1:A:392:ALA:HA	1:A:425:PHE:HB3	1.96	0.48
1:A:394:TRP:CD2	2:A:1626:YX1:HAH3	2.49	0.47
1:A:557:GLU:OE2	1:A:597:ALA:HA	2.14	0.47
1:A:369:GLY:HA3	1:A:372:THR:HG23	1.96	0.47
1:B:51:GLU:HG2	1:B:176:TYR:CZ	2.49	0.47
1:A:150:ASP:OD1	1:A:250:LYS:HD2	2.14	0.47
1:A:98:ASP:OD1	1:A:100:ASN:HA	2.15	0.46
1:B:133:TYR:CE2	1:B:175:ASP:HB3	2.51	0.46
2:B:1626:YX1:OAG	2:B:1626:YX1:H1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:GLU:HA	1:B:230:PRO:HD2	1.80	0.46
1:A:274:PHE:CE2	1:A:313:ARG:HD2	2.50	0.46
1:B:394:TRP:CD2	2:B:1626:YX1:HAH3	2.51	0.46
1:A:177:PRO:HB3	1:A:449:TRP:CE3	2.51	0.45
1:A:339:ALA:O	1:A:347:ARG:HD2	2.15	0.45
1:A:264:ARG:HD2	1:A:269:ALA:HB1	1.98	0.45
1:A:532:MET:HE2	1:A:562:ALA:HB2	1.98	0.45
1:A:358:ASP:HB2	1:A:361:ILE:HD12	1.99	0.45
1:B:133:TYR:HB3	1:B:151:GLY:O	2.17	0.44
1:B:230:PRO:HB3	1:B:283:SER:OG	2.17	0.44
1:A:487:ASN:O	1:A:488:LYS:HB2	2.18	0.44
1:A:98:ASP:CG	1:A:100:ASN:HA	2.44	0.43
1:B:183:GLY:HA3	1:B:212:THR:O	2.18	0.43
1:B:205:TYR:HB3	1:B:210:LEU:HB2	2.00	0.43
1:A:257:ILE:CG2	1:A:294:ILE:HG12	2.48	0.43
1:B:588:GLU:CG	4:B:2223:HOH:O	2.56	0.43
1:A:623:LEU:HD22	1:B:189:TYR:CG	2.54	0.43
1:B:177:PRO:HB3	1:B:449:TRP:CE3	2.54	0.43
1:B:568:SER:O	1:B:571:MET:HB2	2.18	0.43
1:A:138:ASN:HA	1:A:170:GLU:HG2	2.01	0.42
1:A:394:TRP:CD1	1:A:394:TRP:C	2.97	0.42
1:B:619:PHE:CE2	1:B:621:LEU:HG	2.53	0.42
1:A:130:GLU:H	1:A:130:GLU:HG2	1.63	0.42
1:A:510:ASN:ND2	4:A:2183:HOH:O	2.53	0.42
1:A:74:ALA:HB2	1:A:107:GLY:HA2	2.01	0.42
1:A:557:GLU:CG	1:A:602:ALA:HB3	2.46	0.42
1:A:51:GLU:HG2	1:A:176:TYR:CZ	2.55	0.41
1:B:416:ASP:HB3	1:B:419:LEU:HD13	2.02	0.41
1:B:52:ASN:O	1:B:173:ILE:HA	2.20	0.41
1:B:358:ASP:O	1:B:389:ARG:NH2	2.51	0.41
1:A:104:LEU:HD13	1:A:142:ILE:HB	2.01	0.41
1:A:398:PRO:O	1:A:399:VAL:C	2.63	0.41
1:A:109:VAL:C	1:A:111:ASP:H	2.29	0.41
1:B:315:ASN:HA	1:B:319:VAL:HB	2.03	0.40
1:A:54:GLU:O	1:A:171:VAL:HA	2.21	0.40
1:B:366:THR:HA	1:B:394:TRP:O	2.21	0.40
1:B:81:ALA:HA	1:B:84:GLU:HG2	2.02	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	582/594 (98%)	558 (96%)	20 (3%)	4 (1%)	18	19
1	B	582/594 (98%)	562 (97%)	19 (3%)	1 (0%)	43	51
All	All	1164/1188 (98%)	1120 (96%)	39 (3%)	5 (0%)	30	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	301	ASP
1	B	139	ASP
1	A	130	GLU
1	A	608	VAL

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	499/507 (98%)	473 (95%)	26 (5%)	21	26
1	B	499/507 (98%)	468 (94%)	31 (6%)	16	20
All	All	998/1014 (98%)	941 (94%)	57 (6%)	18	23

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	VAL

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Mol	Chain	Res	Type
1	A	61	LYS
1	A	66	ILE
1	A	71	GLU
1	A	86	LEU
1	A	95	SER
1	A	104	LEU
1	A	105	ILE
1	A	121	ASN
1	A	223	HIS
1	A	225	GLU
1	A	257	ILE
1	A	277	LEU
1	A	309	GLN
1	A	313	ARG
1	A	315	ASN
1	A	328	LEU
1	A	365	TRP
1	A	372	THR
1	A	389	ARG
1	A	409	LEU
1	A	488	LYS
1	A	500	GLU
1	A	515	LYS
1	A	545	GLU
1	A	555	LEU
1	B	54	GLU
1	B	66	ILE
1	B	72	GLU
1	B	86	LEU
1	B	96	GLU
1	B	100	ASN
1	B	113	ILE
1	B	118	GLU
1	B	184	ILE
1	B	203	LYS
1	B	223	HIS
1	B	225	GLU
1	B	277	LEU
1	B	279	THR
1	B	287	MET
1	B	299	ILE
1	B	303	SER

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Mol	Chain	Res	Type
1	B	309	GLN
1	B	313	ARG
1	B	328	LEU
1	B	355	GLU
1	B	365	TRP
1	B	389	ARG
1	B	409	LEU
1	B	420	ASN
1	B	500	GLU
1	B	502	ARG
1	B	555	LEU
1	B	557	GLU
1	B	588	GLU
1	B	621	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	121	ASN
1	A	172	ASN
1	A	309	GLN
1	A	421	GLN
1	A	510	ASN
1	A	610	GLN
1	B	47	ASN
1	B	52	ASN
1	B	80	ASN
1	B	167	ASN
1	B	201	GLN
1	B	309	GLN
1	B	315	ASN
1	B	420	ASN
1	B	442	HIS
1	B	542	ASN
1	B	591	GLN
1	B	610	GLN

5.3.3 RNA ⓘ

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](#)

3 ligands are modelled in this entry.

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	SO4	A	1627	-	4,4,4	0.31	0	6,6,6	0.40	0
2	YX1	B	1626	-	17,18,18	1.18	2 (11%)	20,25,25	1.41	3 (15%)
2	YX1	A	1626	-	17,18,18	1.39	3 (17%)	20,25,25	1.26	3 (15%)

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	YX1	B	1626	-	-	2/10/32/32	0/1/1/1
2	YX1	A	1626	-	-	2/10/32/32	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1626	YX1	C1-C2	3.57	1.57	1.52
2	B	1626	YX1	C1-C2	2.65	1.56	1.52
2	A	1626	YX1	O5-C1	2.43	1.48	1.42
2	B	1626	YX1	C2-N2	2.36	1.49	1.45
2	A	1626	YX1	C2-N2	2.01	1.49	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1626	YX1	O5-C5-C4	-3.63	103.15	109.70
2	B	1626	YX1	O5-C1-C2	2.56	112.08	109.52
2	A	1626	YX1	O5-C1-C2	2.18	111.71	109.52
2	A	1626	YX1	OAG-CAM-NAN	2.11	123.49	120.38
2	B	1626	YX1	OAG-CAM-NAN	2.08	123.45	120.38
2	A	1626	YX1	C6-C5-C4	2.08	118.12	113.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

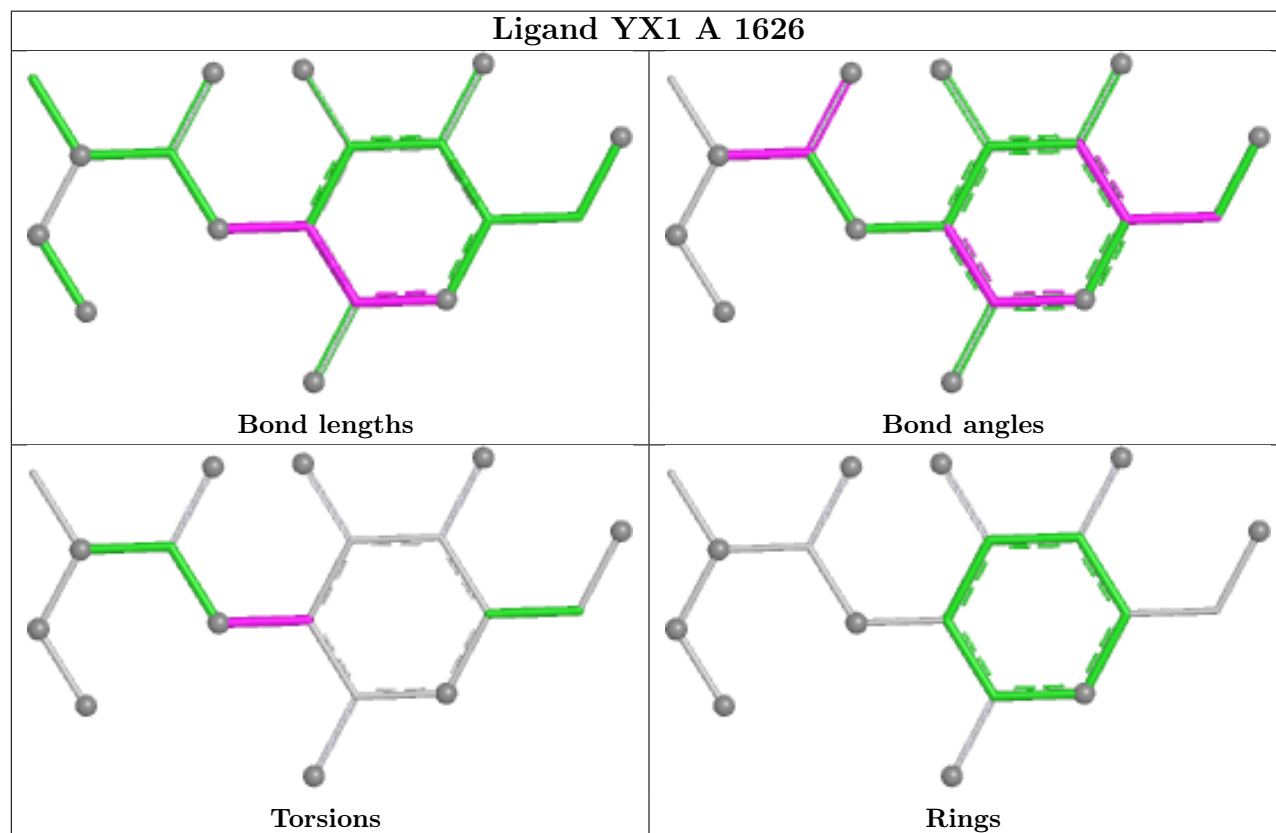
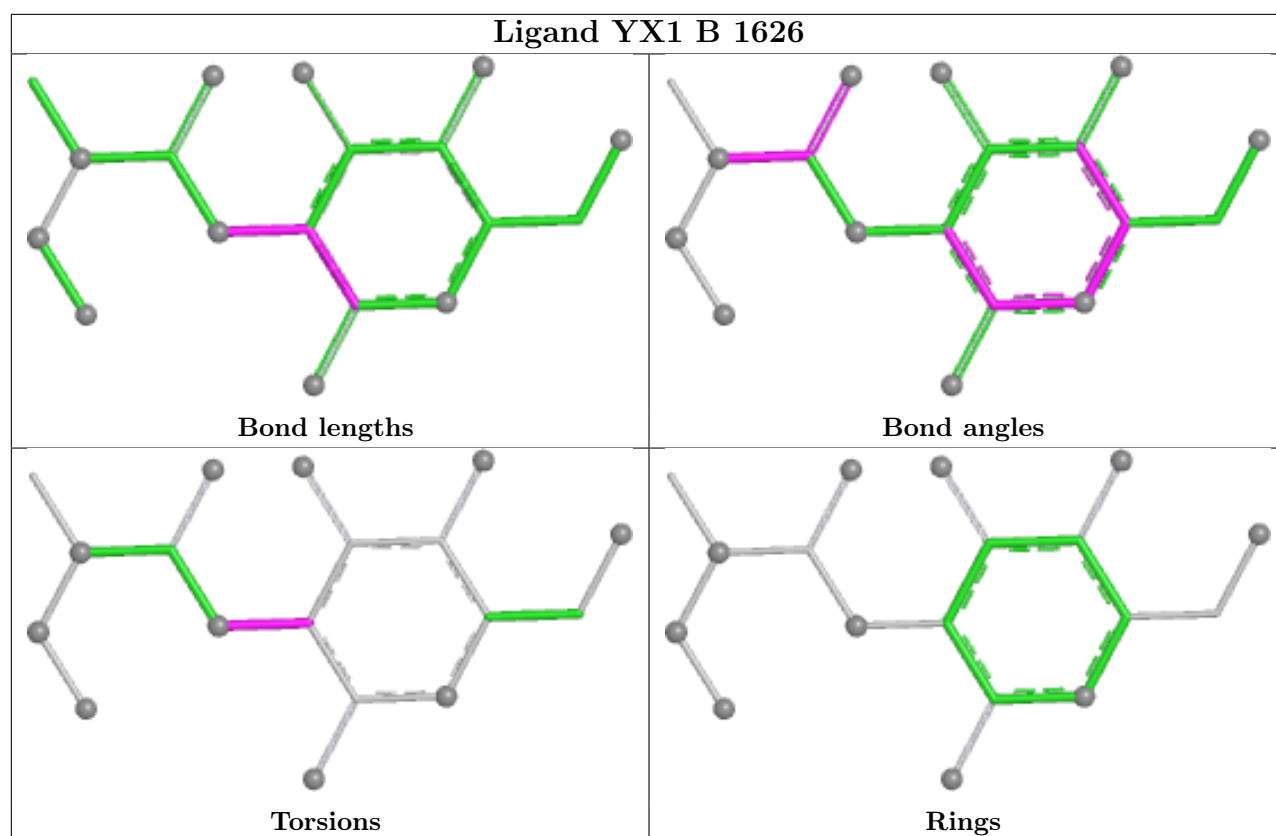
Mol	Chain	Res	Type	Atoms
2	B	1626	YX1	C1-C2-N2-CAM
2	A	1626	YX1	C1-C2-N2-CAM
2	B	1626	YX1	C3-C2-N2-CAM
2	A	1626	YX1	C3-C2-N2-CAM

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1626	YX1	2	0
2	A	1626	YX1	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	584/594 (98%)	0.75	42 (7%) 21 18	23, 43, 54, 66	1 (0%)
1	B	584/594 (98%)	1.10	90 (15%) 5 4	31, 43, 55, 69	0
All	All	1168/1188 (98%)	0.93	132 (11%) 10 8	23, 43, 55, 69	1 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	GLU	9.2
1	A	99	PRO	4.5
1	B	585	SER	4.1
1	A	582	ALA	3.9
1	B	589	ILE	3.9
1	A	110	ASP	3.8
1	B	619	PHE	3.7
1	B	573	VAL	3.6
1	B	616	ALA	3.6
1	B	569	LEU	3.5
1	B	592	ASN	3.5
1	B	618	SER	3.5
1	B	583	TYR	3.5
1	B	309	GLN	3.5
1	B	594	LEU	3.4
1	B	596	THR	3.4
1	B	299	ILE	3.3
1	B	586	ALA	3.3
1	B	609	ALA	3.3
1	B	568	SER	3.2
1	B	582	ALA	3.2
1	A	69	VAL	3.2
1	B	561	LEU	3.2
1	B	575	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	591	GLN	3.1
1	B	572	ILE	3.1
1	A	121	ASN	3.1
1	A	301	ASP	3.1
1	B	624	ILE	2.9
1	B	282	GLU	2.9
1	B	620	ASP	2.9
1	B	41	VAL	2.9
1	B	590	ALA	2.9
1	B	617	LEU	2.9
1	B	301	ASP	2.8
1	A	41	VAL	2.8
1	B	152	THR	2.8
1	B	559	ILE	2.8
1	B	325	VAL	2.8
1	B	580	THR	2.8
1	B	612	PHE	2.8
1	B	613	ILE	2.7
1	B	605	SER	2.7
1	B	518	ALA	2.7
1	B	567	ALA	2.7
1	A	508	LEU	2.7
1	B	103	THR	2.7
1	B	565	ASP	2.7
1	B	122	GLY	2.7
1	A	512	LEU	2.7
1	A	623	LEU	2.7
1	B	521	LEU	2.7
1	B	150	ASP	2.6
1	B	571	MET	2.6
1	B	608	VAL	2.6
1	A	589	ILE	2.6
1	B	562	ALA	2.5
1	A	515	LYS	2.5
1	A	594	LEU	2.5
1	B	621	LEU	2.5
1	B	595	ASN	2.5
1	B	560	THR	2.5
1	B	604	ILE	2.5
1	B	557	GLU	2.5
1	B	576	LEU	2.5
1	B	132	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	601	PHE	2.4
1	A	599	SER	2.4
1	A	587	LYS	2.4
1	B	510	ASN	2.4
1	B	321	ALA	2.4
1	A	585	SER	2.4
1	B	93	ILE	2.4
1	B	318	PHE	2.4
1	A	571	MET	2.4
1	A	81	ALA	2.4
1	B	504	LYS	2.3
1	A	572	ILE	2.3
1	A	573	VAL	2.3
1	B	525	LEU	2.3
1	A	592	ASN	2.3
1	B	597	ALA	2.3
1	B	614	GLN	2.3
1	B	512	LEU	2.3
1	B	537	ASN	2.3
1	A	123	THR	2.3
1	B	356	THR	2.3
1	B	125	ALA	2.2
1	A	580	THR	2.2
1	A	513	SER	2.2
1	B	513	SER	2.2
1	A	93	ILE	2.2
1	B	593	LYS	2.2
1	B	598	LEU	2.2
1	A	109	VAL	2.2
1	B	123	THR	2.2
1	B	535	ALA	2.2
1	A	624	ILE	2.2
1	B	104	LEU	2.2
1	B	128	LEU	2.2
1	A	56	VAL	2.2
1	A	150	ASP	2.2
1	B	114	PRO	2.2
1	B	70	GLY	2.2
1	A	619	PHE	2.1
1	B	529	PHE	2.1
1	B	502	ARG	2.1
1	A	42	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	598	LEU	2.1
1	B	558	LEU	2.1
1	B	588	GLU	2.1
1	B	120	LEU	2.1
1	B	126	GLU	2.1
1	A	510	ASN	2.1
1	A	583	TYR	2.1
1	B	319	VAL	2.1
1	B	403	PHE	2.1
1	B	566	LYS	2.1
1	A	116	LEU	2.1
1	A	569	LEU	2.1
1	A	620	ASP	2.1
1	B	176	TYR	2.1
1	A	107	GLY	2.1
1	B	107	GLY	2.1
1	B	153	PHE	2.1
1	A	561	LEU	2.0
1	B	284	LEU	2.0
1	B	555	LEU	2.0
1	B	564	GLY	2.0
1	A	519	SER	2.0
1	B	101	SER	2.0
1	A	576	LEU	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](#)

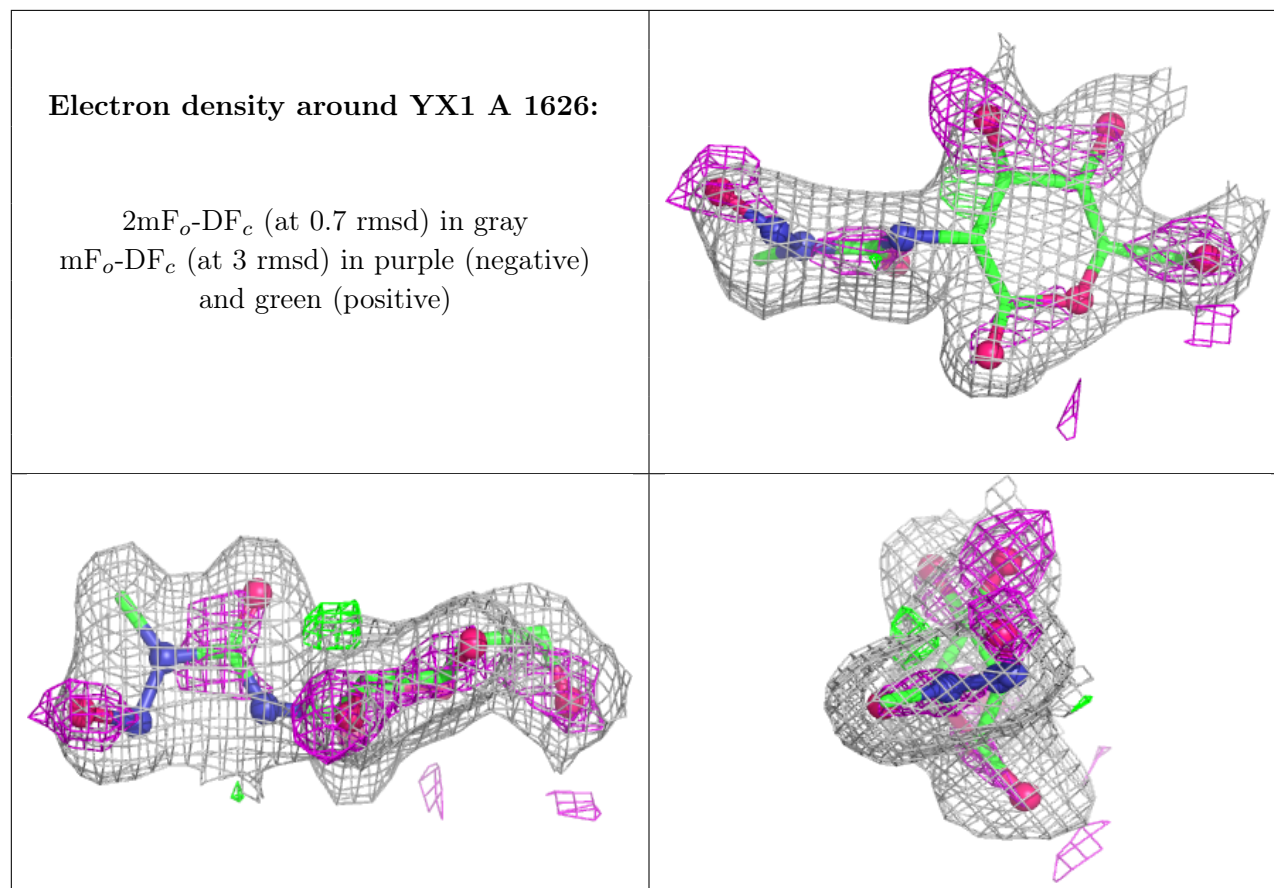
There are no oligosaccharides in this entry.

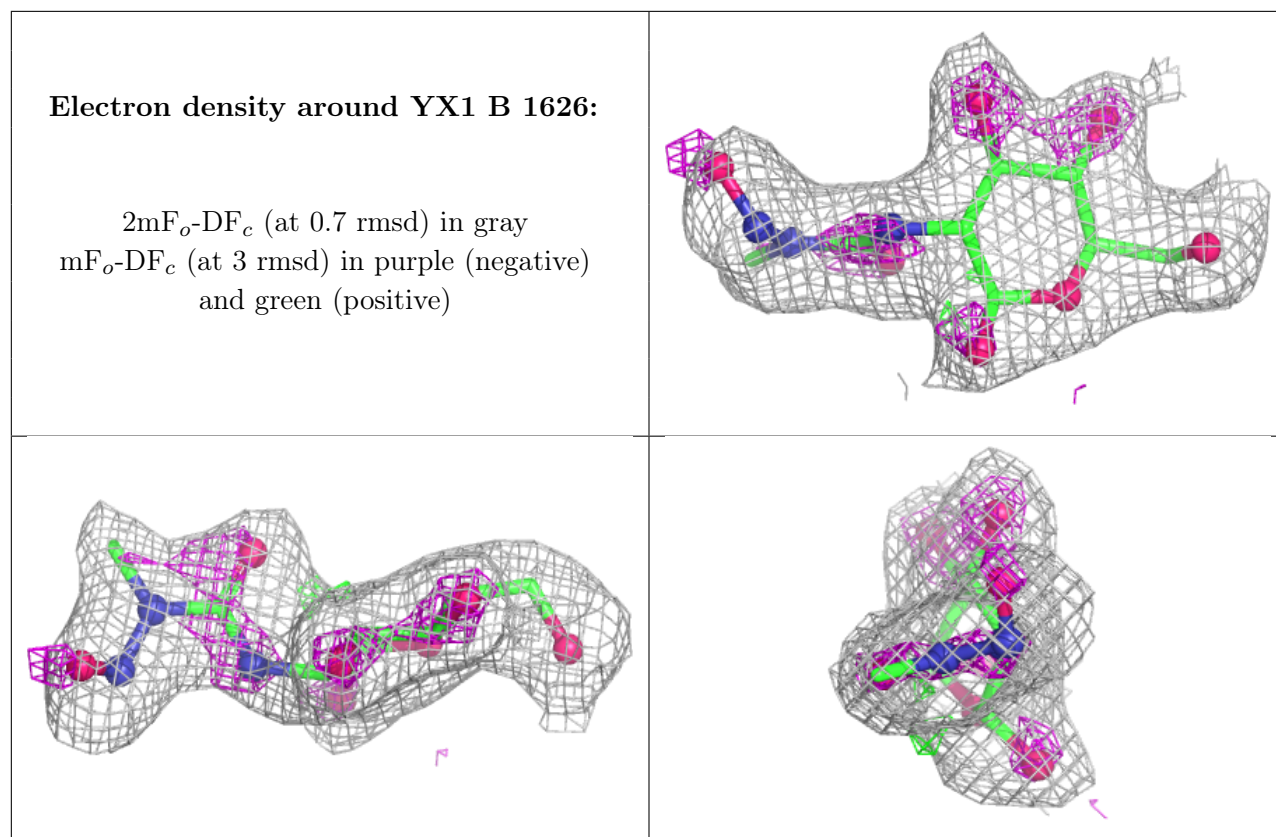
6.4 Ligands [i](#)

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	SO4	A	1627	5/5	0.80	0.19	67,68,69,73	0
2	YX1	A	1626	18/18	0.90	0.10	24,32,38,42	0
2	YX1	B	1626	18/18	0.91	0.09	24,31,36,46	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.