



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:15 AM UTC

PDB ID : 8BVX / pdb_00008bvx
Title : Structure of the mouse 8-oxoguanine DNA Glycosylase mOGG1 in complex with ligand TH13264
Authors : Scaletti, E.; Stenmark, P.
Deposited on : 2022-12-05
Resolution : 2.35 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

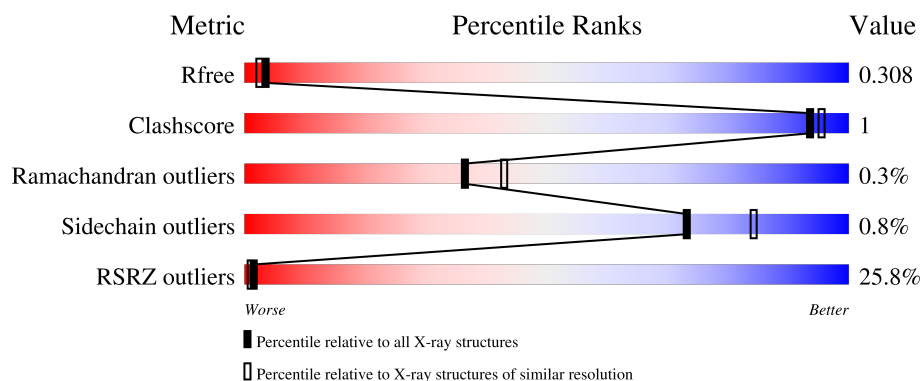
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

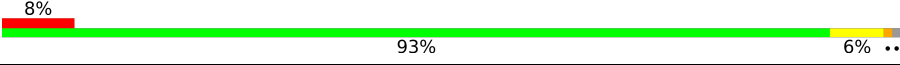
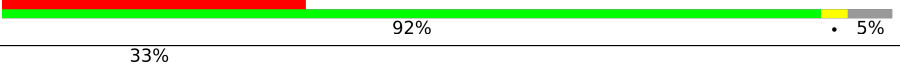
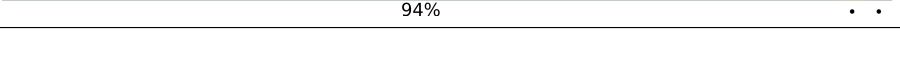
The reported resolution of this entry is 2.35 Å.

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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	318	
1	B	318	
1	C	318	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7423 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.

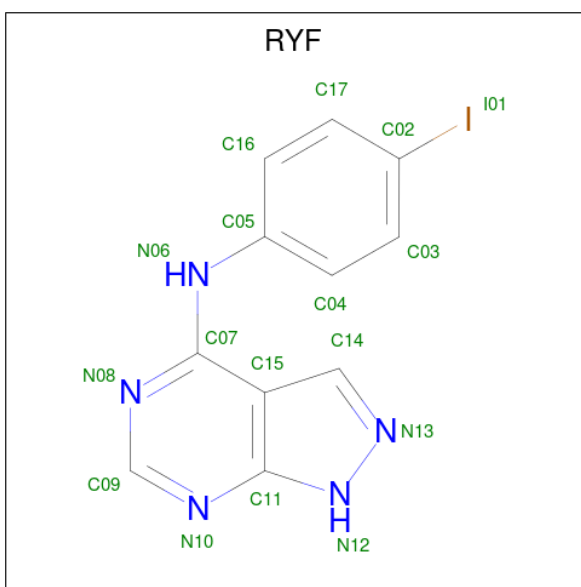
- Molecule 1 is a protein called N-glycosylase/DNA lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2501	1590	452	448	11			
1	B	303	Total	C	N	O	S	0	0	0
			2394	1529	429	425	11			
1	C	307	Total	C	N	O	S	0	0	0
			2395	1531	423	430	11			

There are 6 discrepancies between the modelled and reference sequences:

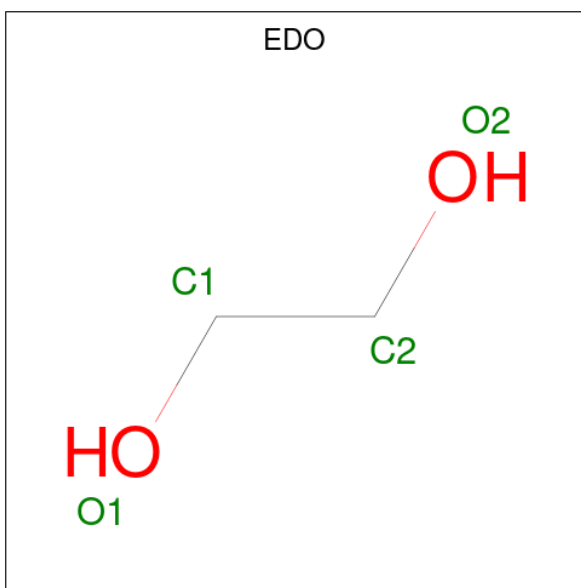
Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLY	-	expression tag	UNP O08760
A	10	HIS	SER	conflict	UNP O08760
B	8	GLY	-	expression tag	UNP O08760
B	10	HIS	SER	conflict	UNP O08760
C	8	GLY	-	expression tag	UNP O08760
C	10	HIS	SER	conflict	UNP O08760

- Molecule 2 is {N}-(4-iodophenyl)-1 {H}-pyrazolo[3,4-d]pyrimidin-4-amine (CCD ID: RYF) (formula: C₁₁H₈IN₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	I	N	0	0
			17	11	1	5		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

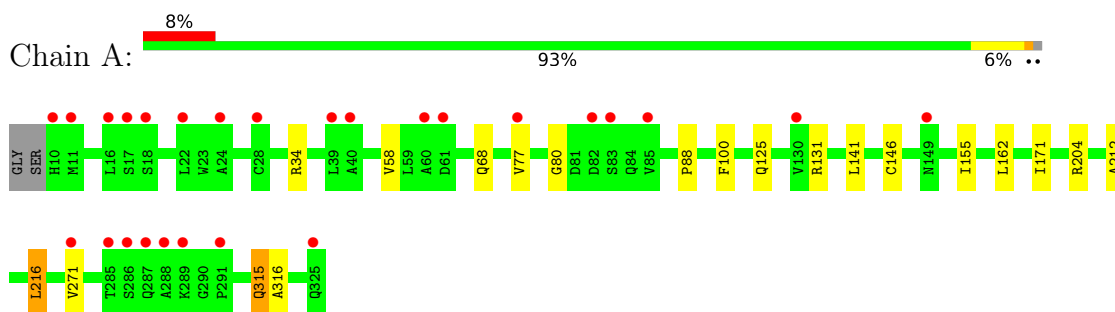
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total 65	O 65	0	0
5	B	25	Total 25	O 25	0	0
5	C	13	Total 13	O 13	0	0

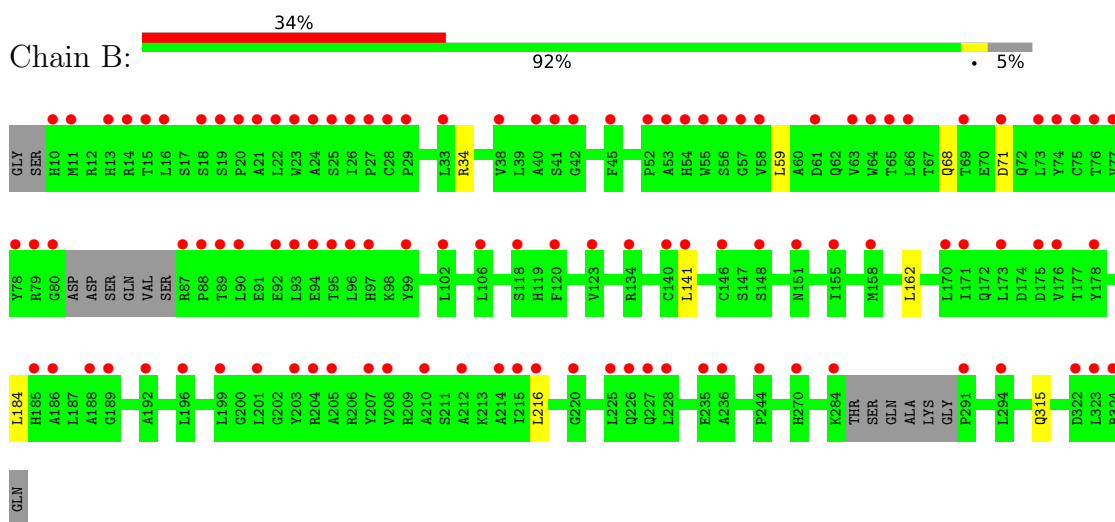
3 Residue-property plots [i](#)

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.

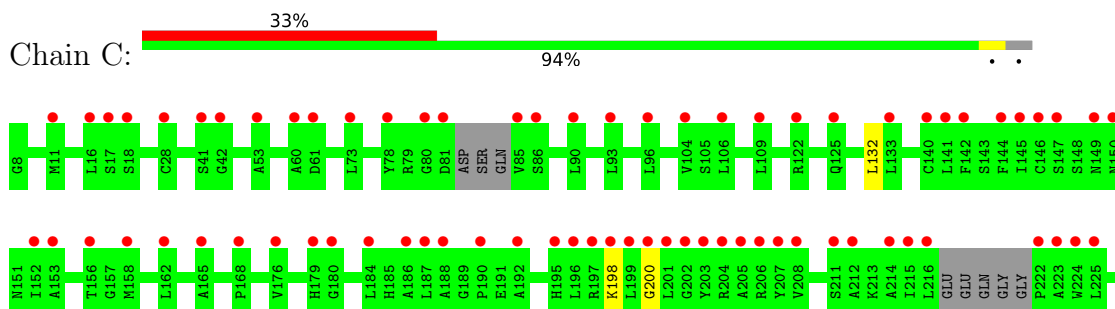
• Molecule 1: N-glycosylase/DNA lyase

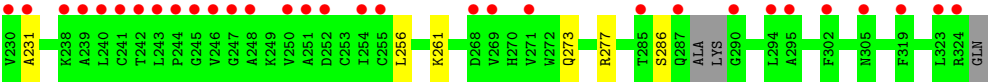


• Molecule 1: N-glycosylase/DNA lyase



• Molecule 1: N-glycosylase/DNA lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.59Å 81.87Å 169.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.85 – 2.35 58.85 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (58.85-2.35) 99.9 (58.85-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.263 , 0.302 0.266 , 0.308	Depositor DCC
R_{free} test set	2387 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7423	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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: NI, EDO, RYF

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	0.45	0/2572	0.78	0/3504
1	B	0.44	0/2462	0.78	0/3352
1	C	0.45	0/2461	0.78	0/3354
All	All	0.45	0/7495	0.78	0/10210

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2501	0	2427	12	0
1	B	2394	0	2326	5	0
1	C	2395	0	2311	3	0
2	A	17	0	0	1	0
3	A	8	0	12	0	0
3	B	4	0	6	0	0
4	A	1	0	0	0	0
5	A	65	0	0	0	0
5	B	25	0	0	0	0
5	C	13	0	0	0	0
All	All	7423	0	7082	20	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 1.

All (20) 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:315:GLN:HE21	1:A:315:GLN:C	2.10	0.59
1:A:77:VAL:HG23	1:A:88:PRO:HG3	1.95	0.49
1:A:80:GLY:HA2	1:A:171:ILE:HD12	1.95	0.48
1:B:162:LEU:C	1:B:162:LEU:HD23	2.38	0.48
1:C:273:GLN:HE21	1:C:277:ARG:HH11	1.61	0.48
1:B:59:LEU:HD13	1:B:59:LEU:C	2.40	0.46
1:A:34:ARG:HA	1:A:68:GLN:HE22	1.82	0.45
1:A:212:ALA:O	1:A:216:LEU:HD22	2.17	0.44
1:A:315:GLN:HE21	1:A:316:ALA:N	2.15	0.44
1:B:184:LEU:HB2	1:B:216:LEU:HD21	2.00	0.44
1:C:132:LEU:HD22	1:C:256:LEU:HG	1.99	0.44
1:A:141:LEU:HD23	1:A:141:LEU:C	2.42	0.44
1:A:146:CYS:HA	1:A:204:ARG:HD3	2.02	0.42
1:A:100:PHE:O	1:A:131:ARG:HD3	2.20	0.42
1:C:231:ALA:O	1:C:261:LYS:NZ	2.51	0.42
1:A:162:LEU:C	1:A:162:LEU:HD23	2.44	0.42
1:A:125:GLN:HE21	1:A:125:GLN:HA	1.86	0.41
1:B:34:ARG:HA	1:B:68:GLN:HE22	1.85	0.41
1:A:155:ILE:HD11	2:A:401:RYF:I01	2.90	0.41
1:B:141:LEU:HD23	1:B:141:LEU:C	2.46	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	314/318 (99%)	306 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	297/318 (93%)	281 (95%)	15 (5%)	1 (0%)	36	43
1	C	299/318 (94%)	282 (94%)	15 (5%)	2 (1%)	18	20
All	All	910/954 (95%)	869 (96%)	38 (4%)	3 (0%)	36	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	200	GLY
1	C	286	SER
1	B	71	ASP

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	261/266 (98%)	257 (98%)	4 (2%)	57	72
1	B	249/266 (94%)	248 (100%)	1 (0%)	84	91
1	C	248/266 (93%)	247 (100%)	1 (0%)	84	91
All	All	758/798 (95%)	752 (99%)	6 (1%)	73	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	VAL
1	A	216	LEU
1	A	271	VAL
1	A	315	GLN
1	B	315	GLN
1	C	198	LYS

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	68	GLN
1	A	125	GLN
1	A	226	GLN
1	A	315	GLN
1	B	68	GLN
1	B	135	GLN
1	B	164	GLN
1	B	219	GLN
1	B	273	GLN
1	B	315	GLN
1	C	62	GLN
1	C	68	GLN
1	C	135	GLN
1	C	150	ASN
1	C	164	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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	401	-	3,3,3	0.07	0	2,2,2	0.14	0
2	RYF	A	401	-	19,19,19	1.57	3 (15%)	22,26,26	4.40	8 (36%)
3	EDO	A	402	-	3,3,3	0.07	0	2,2,2	0.16	0
3	EDO	A	403	-	3,3,3	0.05	0	2,2,2	0.10	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	401	-	-	1/1/1/1	-
2	RYF	A	401	-	-	2/4/4/4	0/3/3/3
3	EDO	A	402	-	-	1/1/1/1	-
3	EDO	A	403	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	RYF	C07-N06	5.25	1.46	1.36
2	A	401	RYF	C15-C11	-2.85	1.37	1.41
2	A	401	RYF	C05-N06	2.33	1.45	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	RYF	C15-C11-N10	-9.54	118.94	126.40
2	A	401	RYF	C11-N12-N13	-9.21	109.11	111.26
2	A	401	RYF	N12-C11-N10	8.82	133.59	125.83
2	A	401	RYF	C15-C14-N13	-8.51	107.79	111.34
2	A	401	RYF	C14-N13-N12	5.65	108.97	106.02
2	A	401	RYF	N10-C09-N08	-4.73	121.43	128.58
2	A	401	RYF	C11-C15-C14	4.46	106.66	104.25
2	A	401	RYF	N06-C07-N08	3.78	122.95	118.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	RYF	N08-C07-N06-C05
3	B	401	EDO	O1-C1-C2-O2

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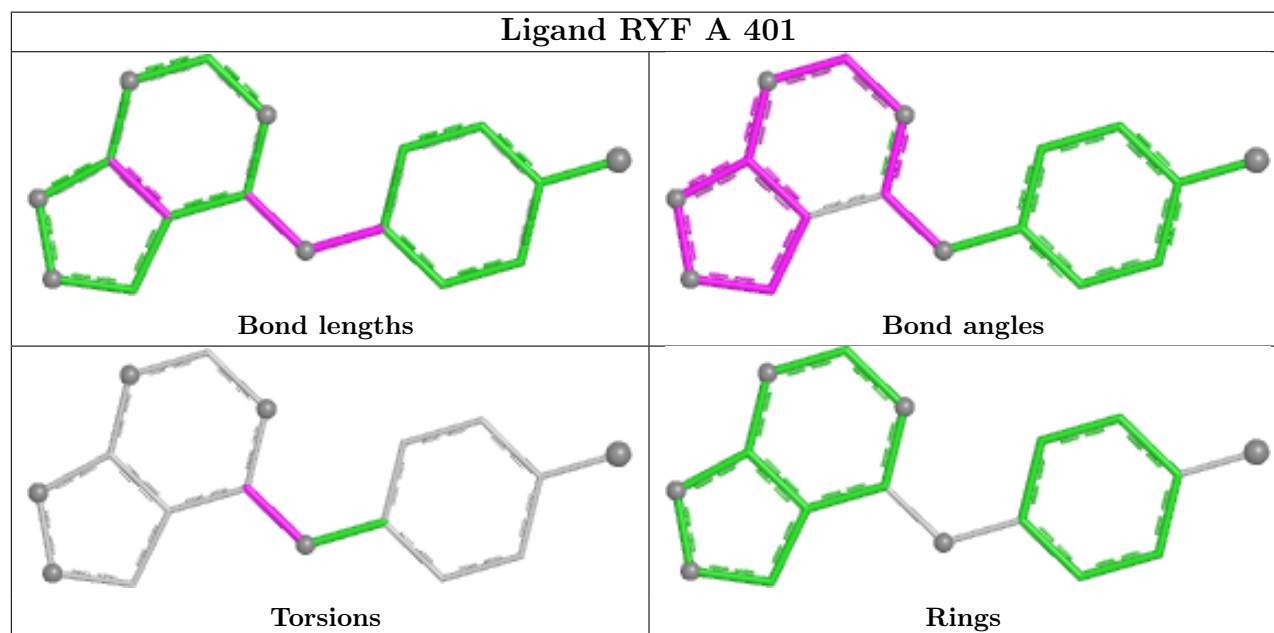
Mol	Chain	Res	Type	Atoms
3	A	403	EDO	O1-C1-C2-O2
2	A	401	RYF	C15-C07-N06-C05
3	A	402	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	RYF	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	316/318 (99%)	0.75	26 (8%)	17 20	37, 54, 91, 116	1 (0%)
1	B	303/318 (95%)	1.74	109 (35%)	1 0	48, 77, 107, 122	0
1	C	307/318 (96%)	1.80	104 (33%)	1 0	50, 82, 121, 140	0
All	All	926/954 (97%)	1.42	239 (25%)	1 1	37, 73, 112, 140	1 (0%)

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	LEU	6.5
1	C	202	GLY	6.2
1	B	93	LEU	6.0
1	B	74	TYR	5.7
1	C	201	LEU	5.6
1	B	16	LEU	5.5
1	B	26	ILE	5.4
1	B	24	ALA	5.3
1	C	162	LEU	5.3
1	C	85	VAL	5.2
1	B	73	LEU	5.2
1	C	203	TYR	4.9
1	C	199	LEU	4.9
1	B	96	LEU	4.7
1	B	77	VAL	4.6
1	B	23	TRP	4.6
1	C	196	LEU	4.5
1	B	25	SER	4.4
1	C	222	PRO	4.4
1	B	69	THR	4.1
1	B	75	CYS	4.0
1	A	288	ALA	4.0
1	B	11	MET	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	289	LYS	3.9
1	C	18	SER	3.9
1	C	224	TRP	3.9
1	A	61	ASP	3.8
1	C	141	LEU	3.8
1	B	225	LEU	3.8
1	C	205	ALA	3.7
1	C	287	GLN	3.7
1	B	207	TYR	3.7
1	B	61	ASP	3.6
1	B	76	THR	3.6
1	C	244	PRO	3.6
1	B	64	TRP	3.6
1	B	78	TYR	3.5
1	C	290	GLY	3.5
1	B	90	LEU	3.5
1	B	324	ARG	3.5
1	A	11	MET	3.5
1	C	225	LEU	3.5
1	B	88	PRO	3.5
1	C	323	LEU	3.5
1	A	285	THR	3.4
1	A	18	SER	3.4
1	B	201	LEU	3.4
1	C	250	VAL	3.4
1	C	188	ALA	3.4
1	C	245	GLY	3.4
1	C	90	LEU	3.3
1	C	187	LEU	3.3
1	B	203	TYR	3.3
1	A	17	SER	3.3
1	B	123	VAL	3.3
1	C	81	ASP	3.3
1	C	106	LEU	3.3
1	C	152	ILE	3.3
1	B	27	PRO	3.3
1	C	208	VAL	3.3
1	C	206	ARG	3.3
1	C	142	PHE	3.2
1	B	185	HIS	3.2
1	C	168	PRO	3.2
1	B	21	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	149	ASN	3.2
1	B	176	VAL	3.2
1	B	28	CYS	3.1
1	C	324	ARG	3.1
1	C	80	GLY	3.1
1	C	150	ASN	3.1
1	B	66	LEU	3.1
1	C	243	LEU	3.1
1	C	104	VAL	3.0
1	C	294	LEU	3.0
1	C	145	ILE	3.0
1	C	247	GLY	3.0
1	C	268	ASP	3.0
1	B	173	LEU	3.0
1	C	146	CYS	2.9
1	B	220	GLY	2.9
1	B	236	ALA	2.9
1	C	197	ARG	2.9
1	A	16	LEU	2.9
1	B	87	ARG	2.9
1	B	216	LEU	2.9
1	B	19	SER	2.9
1	C	86	SER	2.9
1	C	200	GLY	2.9
1	C	207	TYR	2.9
1	B	89	THR	2.9
1	C	240	LEU	2.8
1	C	212	ALA	2.8
1	C	251	ALA	2.8
1	B	63	VAL	2.8
1	B	80	GLY	2.8
1	C	96	LEU	2.8
1	B	15	THR	2.8
1	C	61	ASP	2.8
1	B	33	LEU	2.8
1	C	239	ALA	2.8
1	A	10	HIS	2.8
1	B	97	HIS	2.8
1	C	305	ASN	2.8
1	C	184	LEU	2.8
1	B	171	ILE	2.7
1	A	28	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	241	CYS	2.7
1	B	92	GLU	2.7
1	B	235	GLU	2.7
1	C	109	LEU	2.7
1	C	248	ALA	2.7
1	C	180	GLY	2.7
1	B	29	PRO	2.7
1	C	147	SER	2.7
1	C	140	CYS	2.7
1	A	24	ALA	2.7
1	B	10	HIS	2.7
1	C	153	ALA	2.7
1	C	192	ALA	2.7
1	C	204	ARG	2.7
1	C	186	ALA	2.6
1	C	246	VAL	2.6
1	C	195	HIS	2.6
1	B	53	ALA	2.6
1	B	14	ARG	2.6
1	B	322	ASP	2.6
1	A	85	VAL	2.6
1	B	38	VAL	2.6
1	A	286	SER	2.6
1	B	52	PRO	2.6
1	C	285	THR	2.6
1	C	319	PHE	2.6
1	B	18	SER	2.6
1	B	228	LEU	2.5
1	B	323	LEU	2.5
1	C	16	LEU	2.5
1	C	176	VAL	2.5
1	C	122	ARG	2.5
1	C	93	LEU	2.5
1	C	158	MET	2.5
1	B	42	GLY	2.5
1	B	199	LEU	2.5
1	C	216	LEU	2.5
1	B	55	TRP	2.5
1	C	231	ALA	2.5
1	B	57	GLY	2.5
1	B	291	PRO	2.5
1	C	42	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	190	PRO	2.5
1	B	79	ARG	2.4
1	B	204	ARG	2.4
1	B	120	PHE	2.4
1	C	302	PHE	2.4
1	C	214	ALA	2.4
1	B	65	THR	2.4
1	B	56	SER	2.4
1	A	77	VAL	2.4
1	A	271	VAL	2.4
1	B	45	PHE	2.4
1	A	60	ALA	2.4
1	A	130	VAL	2.4
1	B	58	VAL	2.4
1	C	230	VAL	2.4
1	A	22	LEU	2.4
1	B	141	LEU	2.4
1	A	82	ASP	2.4
1	B	205	ALA	2.4
1	B	210	ALA	2.4
1	C	156	THR	2.4
1	C	133	LEU	2.4
1	B	214	ALA	2.3
1	C	254	ILE	2.3
1	B	13	HIS	2.3
1	B	226	GLN	2.3
1	C	271	VAL	2.3
1	A	39	LEU	2.3
1	B	196	LEU	2.3
1	C	198	LYS	2.3
1	B	215	ILE	2.3
1	C	144	PHE	2.3
1	C	215	ILE	2.3
1	C	73	LEU	2.2
1	B	54	HIS	2.2
1	B	99	TYR	2.2
1	B	118	SER	2.2
1	B	71	ASP	2.2
1	C	252	ASP	2.2
1	B	244	PRO	2.2
1	C	255	CYS	2.2
1	C	165	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	295	ALA	2.2
1	B	178	TYR	2.2
1	C	269	VAL	2.2
1	B	175	ASP	2.2
1	B	158	MET	2.2
1	B	186	ALA	2.2
1	B	148	SER	2.2
1	C	41	SER	2.2
1	B	20	PRO	2.2
1	B	227	GLN	2.2
1	B	294	LEU	2.1
1	B	208	VAL	2.1
1	C	179	HIS	2.1
1	B	189	GLY	2.1
1	A	40	ALA	2.1
1	C	17	SER	2.1
1	B	155	ILE	2.1
1	B	284	LYS	2.1
1	B	146	CYS	2.1
1	B	41	SER	2.1
1	B	188	ALA	2.1
1	B	106	LEU	2.1
1	B	270	HIS	2.1
1	C	125	GLN	2.1
1	A	291	PRO	2.1
1	C	242	THR	2.1
1	B	40	ALA	2.1
1	B	192	ALA	2.1
1	B	212	ALA	2.1
1	C	11	MET	2.1
1	A	287	GLN	2.1
1	A	325	GLN	2.1
1	B	151	ASN	2.1
1	C	78	TYR	2.1
1	C	238	LYS	2.0
1	A	83	SER	2.0
1	C	211	SER	2.0
1	C	28	CYS	2.0
1	C	60	ALA	2.0
1	B	170	LEU	2.0
1	B	94	GLU	2.0
1	B	95	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	53	ALA	2.0
1	C	223	ALA	2.0
1	B	140	CYS	2.0
1	B	102	LEU	2.0
1	C	149	ASN	2.0
1	B	134	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](#)

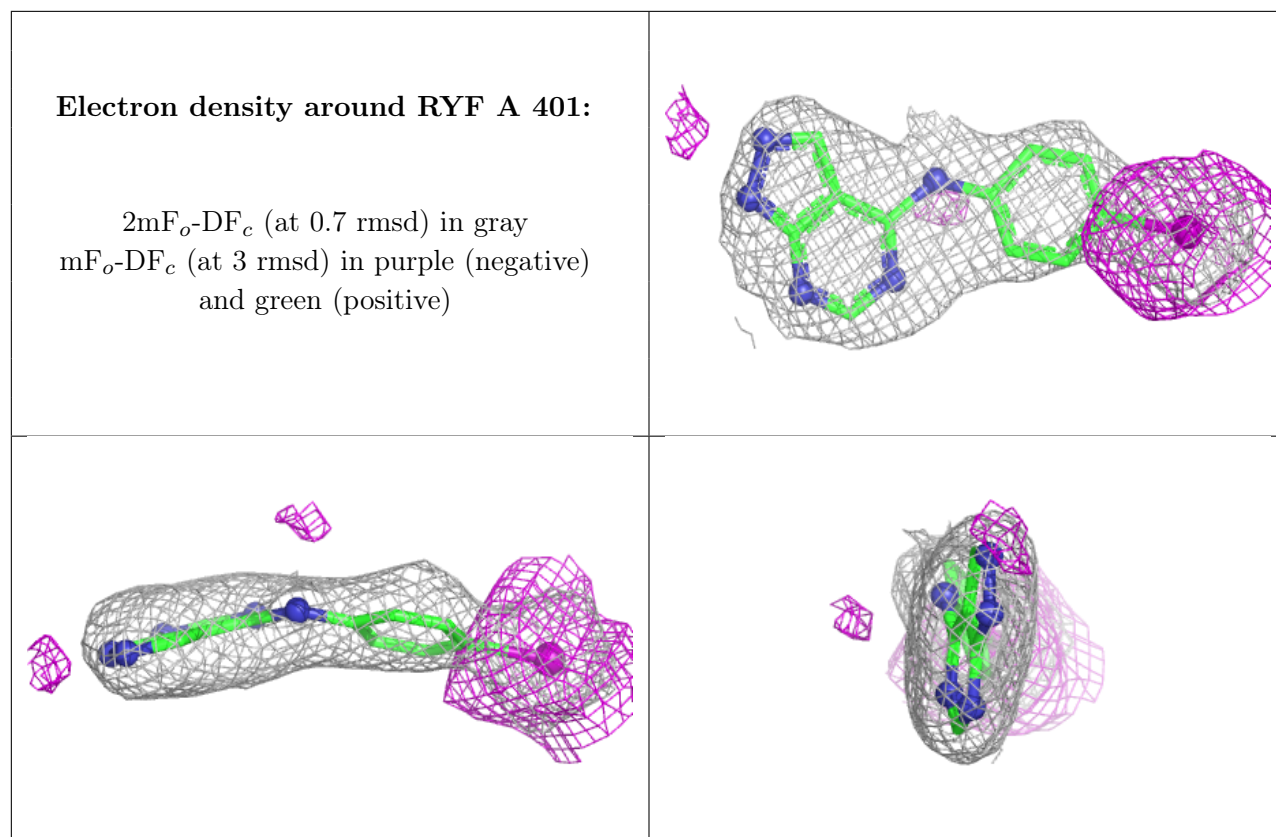
There are no oligosaccharides in this entry.

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	401	4/4	0.65	0.26	83,84,85,85	0
2	RYF	A	401	17/17	0.80	0.20	66,67,106,136	0
3	EDO	A	402	4/4	0.81	0.27	71,72,72,72	0
3	EDO	A	403	4/4	0.90	0.17	64,65,65,66	0
4	NI	A	404	1/1	1.00	0.06	52,52,52,52	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.