



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:01 AM UTC

PDB ID : 2OH4 / pdb_00002oh4
Title : Crystal structure of Vegfr2 with a benzimidazole-urea inhibitor
Authors : Nolte, R.T.; Wang, L.
Deposited on : 2007-01-09
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 ⓘ](#)) 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

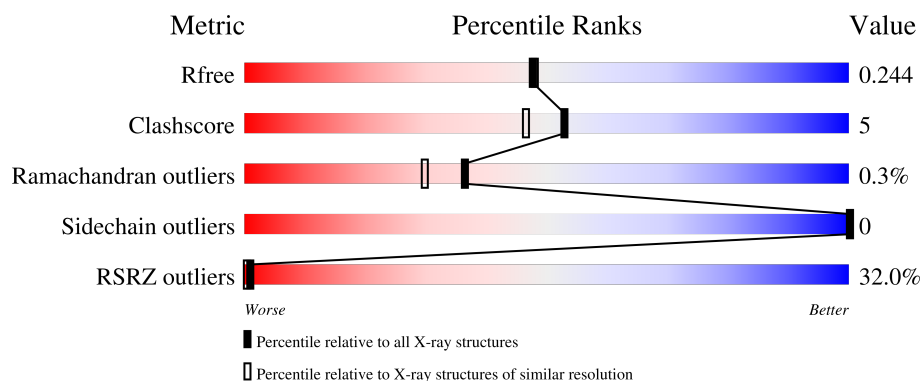
1 Overall quality at a glance

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	316	30% 87% 8% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2661 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.

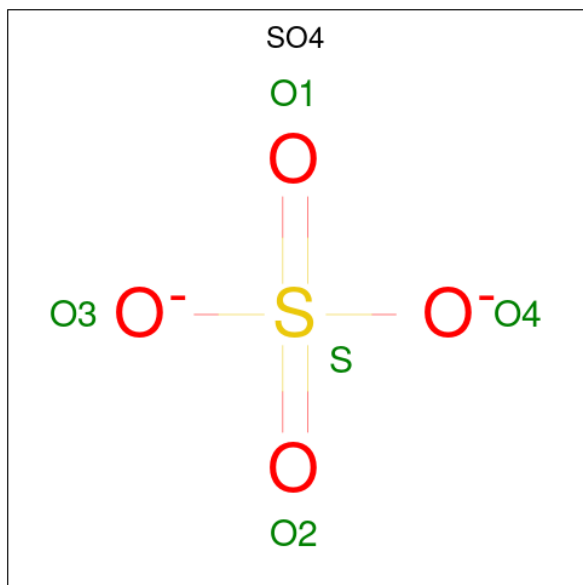
- Molecule 1 is a protein called Vascular endothelial growth factor receptor 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	299	2407	1535	413	438	2	19	0	4	0

There are 2 discrepancies between the modelled and reference sequences:

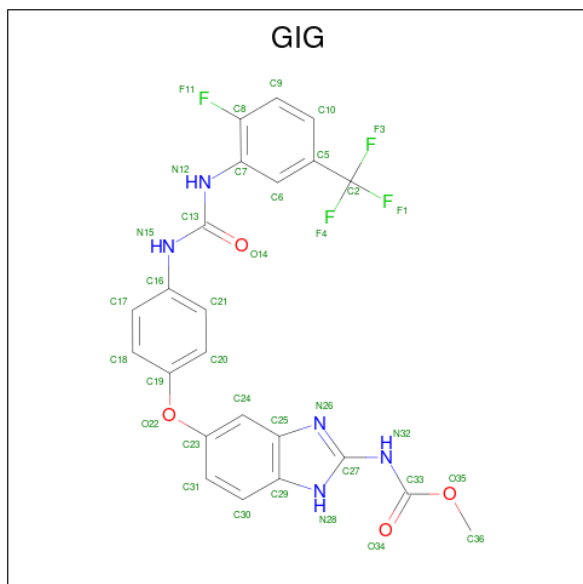
Chain	Residue	Modelled	Actual	Comment	Reference
A	803	HIS	-	expression tag	UNP P35968
A	833	ASN	LYS	conflict	UNP P35968

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is METHYL (5-{4-[(2-FLUORO-5-(TRIFLUOROMETHYL)PHENYL)AMINO]CARBOXYL}AMINO)PHENOXY}-1H-BENZIMIDAZOL-2-YL)CARBAMATE (CCD ID: GIG) (formula: C₂₃H₁₇F₄N₅O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	36	23	4	5	4	0	0

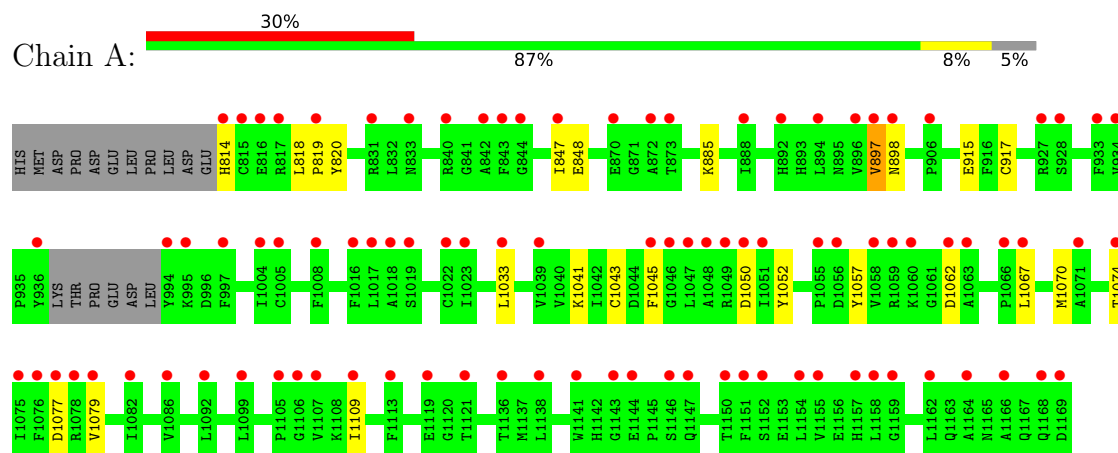
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	208	Total	O	0	0
			208	208		

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: Vascular endothelial growth factor receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	38.37Å 94.25Å 95.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 2.05 47.67 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.67-2.05) 99.5 (47.67-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.04Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.231 0.196 , 0.244	Depositor DCC
R_{free} test set	726 reflections (3.22%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2661	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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: GIG, PTR, SO4

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	0.62	0/2428	0.74	0/3280

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

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	2407	0	2353	23	0
2	A	10	0	0	0	0
3	A	36	0	17	2	0
4	A	208	0	0	5	0
All	All	2661	0	2370	24	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 (24) 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:917:CYS:H	3:A:303:GIG:HN28	1.25	0.81
1:A:1070:MET:HE2	1:A:1074:THR:HG22	1.65	0.79
1:A:897:VAL:HG23	4:A:124:HOH:O	1.86	0.75
1:A:1070:MET:CE	1:A:1074:THR:HG22	2.26	0.66
1:A:898:ASN:HB2	1:A:915:GLU:OE2	2.02	0.60
1:A:819:PRO:HB3	4:A:64:HOH:O	2.02	0.59
1:A:1033:LEU:HD12	1:A:1043[B]:CYS:SG	2.42	0.59
1:A:898:ASN:ND2	4:A:185:HOH:O	2.35	0.59
1:A:1067[B]:LEU:HD23	1:A:1109:ILE:CG2	2.34	0.57
1:A:1067[A]:LEU:HG	4:A:177:HOH:O	2.03	0.57
1:A:1033:LEU:HD21	1:A:1045:PHE:HZ	1.70	0.57
1:A:820:TYR:HB2	1:A:885:LYS:HE2	1.88	0.55
1:A:915:GLU:OE2	1:A:1041:LYS:HD3	2.09	0.52
1:A:1050:ASP:OD2	1:A:1062:ASP:O	2.27	0.52
1:A:1067[B]:LEU:HD23	1:A:1109:ILE:HG22	1.91	0.52
1:A:1077:ASP:HB2	1:A:1079:VAL:HG23	1.92	0.52
1:A:1070:MET:HE1	4:A:176:HOH:O	2.11	0.50
1:A:1067[B]:LEU:CD2	1:A:1109:ILE:HG22	2.44	0.48
1:A:814:HIS:CB	1:A:818:LEU:HD11	2.46	0.44
1:A:1067[B]:LEU:HD23	1:A:1109:ILE:HG21	1.99	0.44
1:A:1033:LEU:CD1	1:A:1043[B]:CYS:SG	3.07	0.43
1:A:1067[B]:LEU:CD2	1:A:1109:ILE:CG2	2.96	0.42
1:A:847:ILE:HG22	1:A:848:GLU:O	2.19	0.42
3:A:303:GIG:H6	3:A:303:GIG:O14	2.20	0.42

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	297/316 (94%)	287 (97%)	9 (3%)	1 (0%)	36 30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	897	VAL

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	253/274 (92%)	253 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	877	HIS
1	A	1147	GLN
1	A	1157	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	PTR	A	1052	1	15,16,17	1.91	1 (6%)	17,22,24	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PTR	A	1057	1	15,16,17	2.02	1 (6%)	17,22,24	0.47	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
1	PTR	A	1052	1	-	1/10/11/13	0/1/1/1
1	PTR	A	1057	1	-	1/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1057	PTR	OH-CZ	-7.66	1.23	1.40
1	A	1052	PTR	OH-CZ	-7.23	1.24	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1052	PTR	C-CA-CB-CG
1	A	1057	PTR	CZ-OH-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

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	GIG	A	303	-	39,39,39	1.48	3 (7%)	56,56,56	1.25	4 (7%)
2	SO4	A	302	-	4,4,4	0.24	0	6,6,6	0.06	0
2	SO4	A	301	-	4,4,4	0.20	0	6,6,6	0.20	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	GIG	A	303	-	-	4/24/24/24	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	GIG	C27-N26	5.42	1.41	1.32
3	A	303	GIG	C29-C25	3.14	1.44	1.40
3	A	303	GIG	O34-C33	2.81	1.26	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	GIG	O35-C33-O34	-4.63	117.88	124.62
3	A	303	GIG	C25-C29-N28	3.45	109.86	105.71
3	A	303	GIG	C31-C23-C24	2.36	123.68	120.50
3	A	303	GIG	C29-C25-N26	-2.06	106.60	109.42

There are no chirality outliers.

All (4) torsion outliers are listed below:

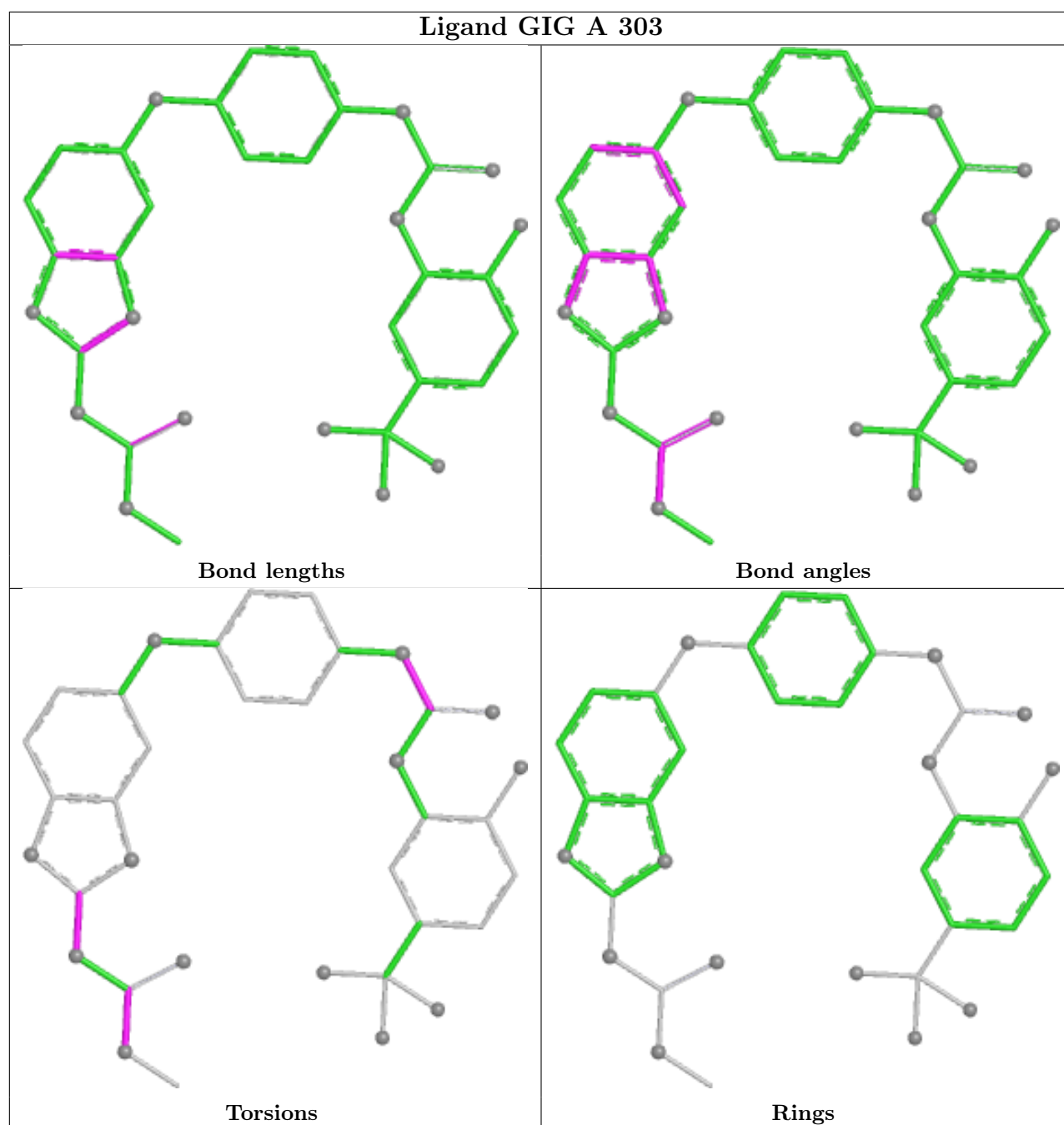
Mol	Chain	Res	Type	Atoms
3	A	303	GIG	O34-C33-O35-C36
3	A	303	GIG	O14-C13-N15-C16
3	A	303	GIG	N26-C27-N32-C33
3	A	303	GIG	N28-C27-N32-C33

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	GIG	2	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	297/316 (93%)	1.66	95 (31%) 1 0	26, 54, 68, 73	4 (1%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	815	CYS	5.3
1	A	872	ALA	5.0
1	A	1047	LEU	4.9
1	A	816	GLU	4.6
1	A	1059	ARG	4.6
1	A	936	TYR	4.4
1	A	843	PHE	4.3
1	A	1076	PHE	4.3
1	A	1046	GLY	4.1
1	A	897	VAL	4.0
1	A	833	ASN	3.9
1	A	1056	ASP	3.9
1	A	1048	ALA	3.9
1	A	1078	ARG	3.8
1	A	1050	ASP	3.7
1	A	1168	GLN	3.7
1	A	1022	CYS	3.5
1	A	1018	ALA	3.5
1	A	1067[A]	LEU	3.5
1	A	906	PRO	3.4
1	A	1169	ASP	3.4
1	A	1045	PHE	3.3
1	A	1107	VAL	3.2
1	A	997	PHE	3.2
1	A	1155	VAL	3.2
1	A	1055	PRO	3.2
1	A	817	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	870	GLU	3.1
1	A	1075	ILE	3.1
1	A	1060	LYS	3.1
1	A	994	TYR	3.1
1	A	1147	GLN	3.1
1	A	934	VAL	3.1
1	A	1158	LEU	3.0
1	A	1058	VAL	2.8
1	A	1150	THR	2.8
1	A	927	ARG	2.8
1	A	995	LYS	2.7
1	A	1077	ASP	2.7
1	A	1079	VAL	2.7
1	A	1062	ASP	2.7
1	A	1063	ALA	2.7
1	A	1066	PRO	2.6
1	A	844	GLY	2.6
1	A	1051	ILE	2.6
1	A	1159	GLY	2.6
1	A	1141	TRP	2.6
1	A	1113	PHE	2.6
1	A	888	ILE	2.6
1	A	1109	ILE	2.6
1	A	842	ALA	2.6
1	A	1016	PHE	2.5
1	A	892	HIS	2.5
1	A	1144	GLU	2.5
1	A	1164	ALA	2.5
1	A	1017	LEU	2.5
1	A	1138	LEU	2.4
1	A	894	LEU	2.4
1	A	840	ARG	2.4
1	A	1086	VAL	2.4
1	A	1105	PRO	2.4
1	A	1162	LEU	2.3
1	A	1151	PHE	2.3
1	A	1152	SER	2.3
1	A	819	PRO	2.3
1	A	1166	ALA	2.3
1	A	1143	GLY	2.3
1	A	1019	SER	2.3
1	A	1099	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	933	PHE	2.2
1	A	1008	PHE	2.2
1	A	847	ILE	2.2
1	A	1136	THR	2.2
1	A	1121	THR	2.2
1	A	1005	CYS	2.2
1	A	1023	ILE	2.2
1	A	814	HIS	2.2
1	A	1033	LEU	2.2
1	A	1154	LEU	2.2
1	A	1074	THR	2.2
1	A	1106	GLY	2.1
1	A	1157	HIS	2.1
1	A	1092	LEU	2.1
1	A	1146	SER	2.1
1	A	873	THR	2.1
1	A	1082	ILE	2.1
1	A	896	VAL	2.1
1	A	831	ARG	2.0
1	A	1004	ILE	2.0
1	A	1039	VAL	2.0
1	A	1119	GLU	2.0
1	A	928	SER	2.0
1	A	1071	ALA	2.0
1	A	898	ASN	2.0
1	A	1049	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PTR	A	1057	16/17	0.61	0.20	65,66,68,69	0
1	PTR	A	1052	16/17	0.77	0.17	65,66,71,72	0

6.3 Carbohydrates [i](#)

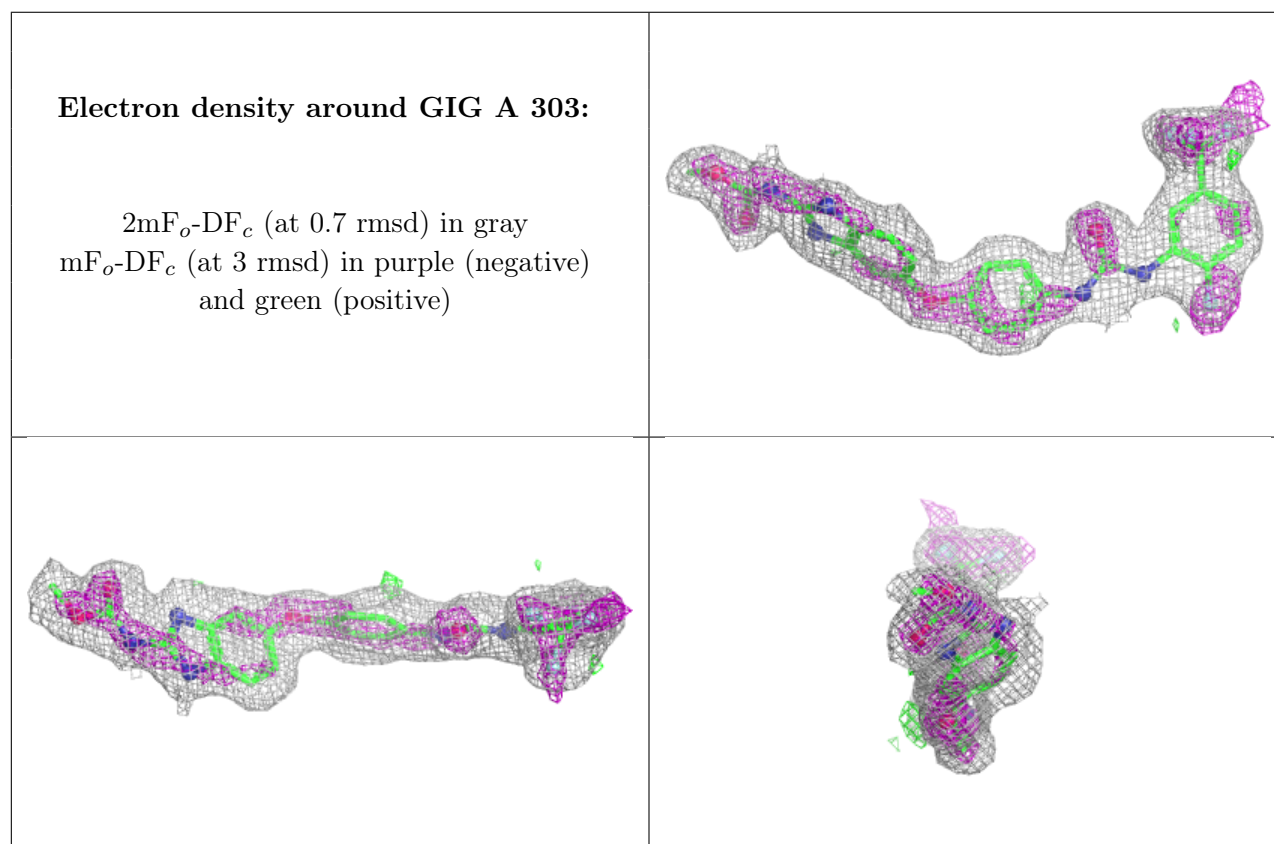
There are no oligosaccharides in this entry.

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
2	SO4	A	302	5/5	0.40	0.17	154,154,154,154	0
2	SO4	A	301	5/5	0.65	0.19	75,75,77,77	0
3	GIG	A	303	36/36	0.93	0.12	36,39,46,50	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.