



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:47 PM UTC

PDB ID : 9U7E / pdb_00009u7e
Title : FGFR2 kinase domain with a macrocyclic compound 8g
Authors : Chen, X.J.; Chen, Y.H.
Deposited on : 2025-03-24
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

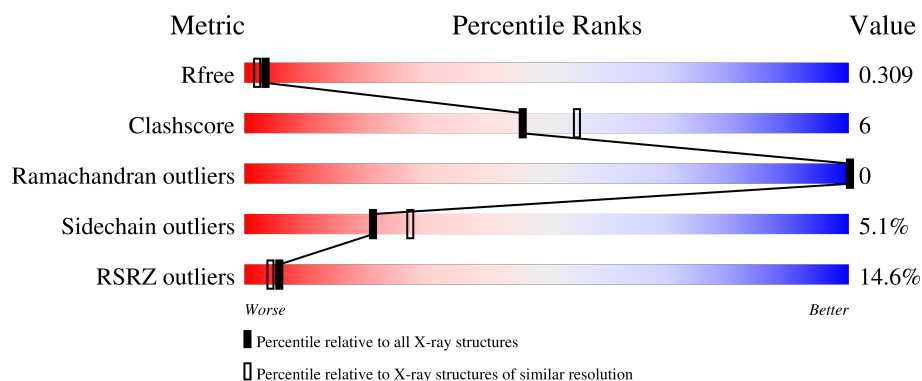
1 Overall quality at a glance

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	304	15% 81% 13% • 5%
1	B	304	12% 73% 17% • 7%

2 Entry composition [i](#)

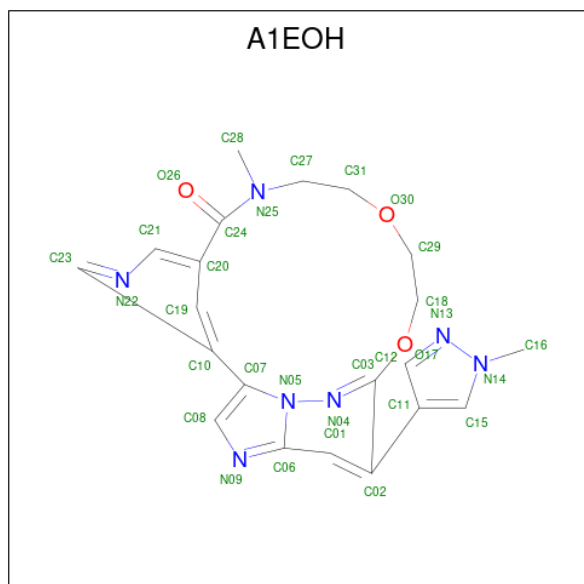
There are 4 unique types of molecules in this entry. The entry contains 4653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	1	0
			2243	1430	378	413	22			
1	B	282	Total	C	N	O	S	0	1	0
			2192	1397	371	402	22			

- Molecule 2 is (E)-4-methyl-17-(1-methyl-1H-pyrazol-4-yl)-7,10-dioxo-4-aza-1(3,6)-imidazo[1,2-b]pyridazina-2(3,5)-pyridinacyclodecaphan-3-one (CCD ID: A1EOH) (formula: C₂₁H₂₁N₇O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	21	7	3		
2	B	1	Total	C	N	O	0	0
			31	21	7	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

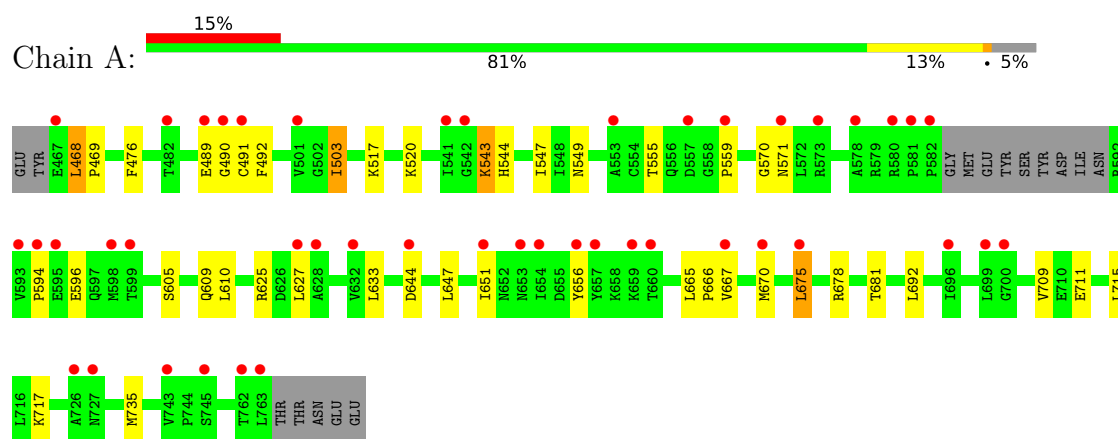
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	75	Total	O	0	0
			75	75		

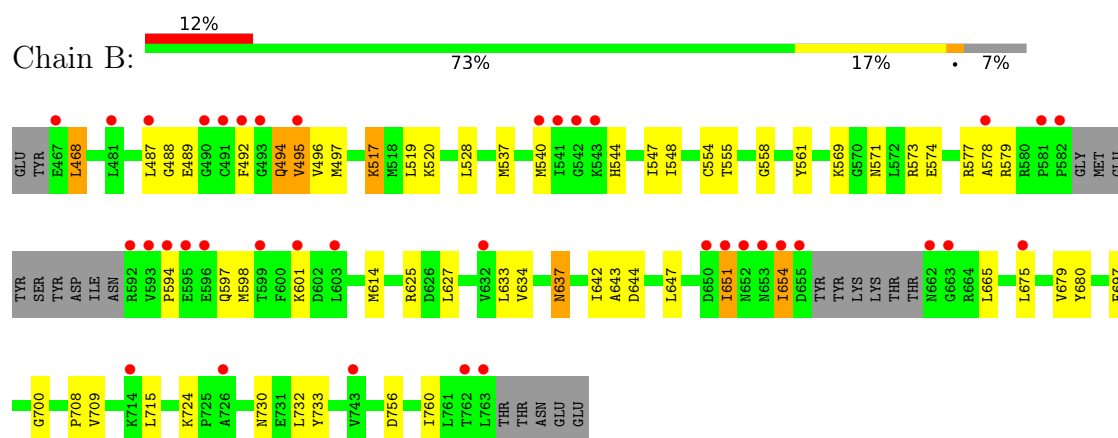
3 Residue-property plots [i](#)

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: Fibroblast growth factor receptor 2



• Molecule 1: Fibroblast 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	66.94Å 77.35Å 115.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.66 – 2.20 57.66 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (57.66-2.20) 99.3 (57.66-2.20)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.260 , 0.312 0.262 , 0.309	Depositor DCC
R_{free} test set	2000 reflections (6.43%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.749	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4653	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2503e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, A1EOH

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	0.42	1/2292 (0.0%)	0.50	3/3111 (0.1%)
1	B	0.66	5/2238 (0.2%)	0.60	2/3034 (0.1%)
All	All	0.55	6/4530 (0.1%)	0.55	5/6145 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	730	ASN	C-O	-6.40	1.16	1.24
1	A	555	THR	C-O	-5.86	1.16	1.23
1	B	488	GLY	C-O	-5.80	1.17	1.24
1	B	644	ASP	C-O	-5.42	1.17	1.24
1	B	574	GLU	C-O	-5.39	1.17	1.24
1	B	495	VAL	C-O	-5.10	1.18	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	644	ASP	N-CA-C	7.90	120.15	110.91
1	A	490	GLY	CA-C-N	6.03	130.25	120.60
1	A	490	GLY	C-N-CA	6.03	130.25	120.60
1	B	651	ILE	N-CA-C	5.39	114.96	108.06
1	B	644	ASP	N-CA-C	5.32	122.12	110.80

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	2243	0	2186	21	0
1	B	2192	0	2145	32	0
2	A	31	0	0	0	0
2	B	31	0	0	1	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	71	0	0	2	0
4	B	75	0	0	0	0
All	All	4653	0	4331	51	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 6.

All (51) 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:487:LEU:HD21	1:B:497:MET:HB2	1.63	0.81
1:A:656:TYR:O	1:A:678:ARG:NH1	2.29	0.66
1:B:492:PHE:HE1	1:B:495:VAL:HG12	1.61	0.66
1:B:579:ARG:HB3	1:B:597:GLN:HA	1.81	0.63
1:B:544:HIS:HB3	1:B:547:ILE:HD12	1.82	0.60
1:B:637:ASN:OD1	1:B:637:ASN:N	2.32	0.60
1:B:573:ARG:NH1	1:B:700:GLY:O	2.34	0.60
1:B:554:CYS:HB2	1:B:561:TYR:HB2	1.83	0.60
1:B:579:ARG:HD3	1:B:598:MET:HE3	1.84	0.59
1:A:571:ASN:ND2	4:A:901:HOH:O	2.23	0.58
1:B:494:GLN:HG3	1:B:520:LYS:HG2	1.85	0.58
1:A:610:LEU:HD13	1:A:692:LEU:HD21	1.89	0.55
1:B:724:LYS:HB2	1:B:733:TYR:CD2	2.44	0.53
1:A:492:PHE:HB2	1:A:517:LYS:HE3	1.92	0.51
1:B:492:PHE:CE1	1:B:495:VAL:HG12	2.43	0.51
1:A:520:LYS:NZ	4:A:910:HOH:O	2.42	0.51
1:B:519:LEU:HD11	1:B:528:LEU:HD13	1.93	0.50
1:A:559:PRO:HD3	1:B:708:PRO:HG3	1.94	0.49
1:B:569:LYS:HB2	1:B:634:VAL:HB	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:HIS:HB3	1:A:547:ILE:HD12	1.94	0.48
1:B:468:LEU:HD13	1:B:555:THR:HB	1.96	0.48
1:B:697:PHE:CZ	1:B:732:LEU:HD13	2.48	0.48
1:B:724:LYS:HB2	1:B:733:TYR:CG	2.49	0.47
1:B:489:GLU:HG3	1:B:494:GLN:HG2	1.96	0.47
1:A:594:PRO:O	1:A:596:GLU:N	2.47	0.47
1:A:665:LEU:HD13	1:A:670:MET:HE2	1.96	0.47
1:B:578:ALA:HB1	1:B:594:PRO:HD2	1.97	0.47
1:A:543:LYS:HA	1:A:549:ASN:OD1	2.15	0.47
1:A:711:GLU:OE2	1:B:558:GLY:HA2	2.14	0.46
1:B:487:LEU:HD13	2:B:801:A1EOH:C01	2.45	0.46
1:B:537:MET:HE3	1:B:540:MET:HB2	1.98	0.46
1:B:577:ARG:NH2	3:B:802:SO4:O2	2.49	0.46
1:A:605:SER:O	1:A:609:GLN:HG3	2.18	0.44
1:B:492:PHE:O	1:B:517:LYS:HD2	2.16	0.43
1:A:735:MET:HE3	1:A:735:MET:HB2	1.88	0.43
1:B:614:MET:SD	1:B:642:ILE:HD13	2.58	0.43
1:A:670:MET:HB2	1:A:675:LEU:HD13	2.00	0.43
1:B:756:ASP:O	1:B:760:ILE:HG13	2.19	0.42
1:A:666:PRO:O	1:A:670:MET:HG2	2.18	0.42
1:A:543:LYS:HE3	1:A:544:HIS:N	2.35	0.42
1:A:476:PHE:CD1	1:A:503:ILE:HD12	2.54	0.42
1:B:625:ARG:HD3	1:B:647:LEU:O	2.20	0.42
1:B:654:ILE:CG2	1:B:679:VAL:HB	2.50	0.41
1:B:548:ILE:HG13	1:B:643:ALA:HB2	2.03	0.41
1:A:651:ILE:HD11	1:A:681:THR:HA	2.02	0.41
1:A:570:GLY:O	1:A:633:LEU:HA	2.21	0.41
1:A:625:ARG:HD3	1:A:647:LEU:O	2.21	0.41
1:B:627:LEU:HD23	1:B:627:LEU:HA	1.92	0.41
1:A:468:LEU:HA	1:A:469:PRO:HD3	1.93	0.40
1:B:548:ILE:HG13	1:B:633:LEU:HD12	2.03	0.40
1:B:625:ARG:HA	1:B:680:TYR:OH	2.22	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	285/304 (94%)	277 (97%)	8 (3%)	0	100	100
1	B	277/304 (91%)	268 (97%)	9 (3%)	0	100	100
All	All	562/608 (92%)	545 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	237/268 (88%)	226 (95%)	11 (5%)	24	32
1	B	232/268 (87%)	219 (94%)	13 (6%)	19	24
All	All	469/536 (88%)	445 (95%)	24 (5%)	21	27

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	468	LEU
1	A	489	GLU
1	A	491	CYS
1	A	503	ILE
1	A	543	LYS
1	A	627	LEU
1	A	667	VAL
1	A	675	LEU
1	A	709	VAL
1	A	715	LEU
1	A	717	LYS
1	B	468	LEU
1	B	494	GLN
1	B	496	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	517	LYS
1	B	571	ASN
1	B	601	LYS
1	B	637	ASN
1	B	651	ILE
1	B	654	ILE
1	B	665	LEU
1	B	675	LEU
1	B	709	VAL
1	B	715	LEU

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	494	GLN
1	A	556	GLN
1	B	730	ASN

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](#)

4 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	802	-	4,4,4	0.45	0	6,6,6	0.95	0
2	A1EOH	B	801	-	35,35,35	2.31	9 (25%)	40,50,50	2.89	9 (22%)
2	A1EOH	A	801	-	35,35,35	2.29	8 (22%)	40,50,50	2.82	11 (27%)
3	SO4	B	802	-	4,4,4	0.40	0	6,6,6	0.79	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
2	A1EOH	B	801	-	-	9/24/25/25	0/3/5/5
2	A1EOH	A	801	-	-	8/24/25/25	0/3/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	A1EOH	C06-N05	-6.91	1.29	1.39
2	B	801	A1EOH	C24-N25	6.88	1.46	1.34
2	B	801	A1EOH	C06-N05	-6.80	1.29	1.39
2	A	801	A1EOH	C24-N25	6.78	1.45	1.34
2	A	801	A1EOH	C02-C11	4.31	1.53	1.47
2	B	801	A1EOH	C02-C11	3.72	1.52	1.47
2	B	801	A1EOH	O17-C03	3.68	1.42	1.34
2	A	801	A1EOH	O17-C03	3.50	1.41	1.34
2	B	801	A1EOH	C15-N14	-3.14	1.30	1.34
2	B	801	A1EOH	C10-C07	2.98	1.52	1.48
2	A	801	A1EOH	C15-N14	-2.96	1.31	1.34
2	A	801	A1EOH	C10-C07	2.75	1.52	1.48
2	A	801	A1EOH	C08-N09	-2.66	1.32	1.37
2	B	801	A1EOH	C08-N09	-2.48	1.32	1.37
2	B	801	A1EOH	N14-N13	-2.31	1.33	1.35
2	B	801	A1EOH	C06-N09	2.25	1.36	1.33
2	A	801	A1EOH	N14-N13	-2.23	1.33	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	A1EOH	C12-N13-N14	11.56	110.76	104.41
2	A	801	A1EOH	C12-N13-N14	10.66	110.26	104.41
2	A	801	A1EOH	C16-N14-N13	6.74	125.43	120.03
2	B	801	A1EOH	C16-N14-N13	6.67	125.38	120.03
2	B	801	A1EOH	C11-C12-N13	-6.53	106.90	112.09
2	A	801	A1EOH	C11-C12-N13	-5.95	107.36	112.09
2	A	801	A1EOH	C06-N05-N04	-4.96	121.83	126.75
2	B	801	A1EOH	C06-N05-N04	-4.55	122.25	126.75
2	B	801	A1EOH	C15-N14-N13	-3.84	109.90	112.08
2	A	801	A1EOH	C08-N09-C06	3.74	107.61	105.11
2	A	801	A1EOH	C15-N14-N13	-3.56	110.06	112.08
2	A	801	A1EOH	C16-N14-C15	-3.42	124.51	127.94
2	A	801	A1EOH	C07-C08-N09	-3.29	108.83	112.37
2	B	801	A1EOH	C07-C08-N09	-3.22	108.90	112.37
2	B	801	A1EOH	C16-N14-C15	-3.21	124.72	127.94
2	B	801	A1EOH	C08-N09-C06	2.87	107.03	105.11
2	A	801	A1EOH	C23-N22-C21	2.80	121.31	117.51
2	B	801	A1EOH	C23-N22-C21	2.71	121.19	117.51
2	A	801	A1EOH	C18-O17-C03	-2.26	112.54	117.14
2	A	801	A1EOH	O26-C24-N25	-2.20	118.50	122.21

There are no chirality outliers.

All (17) torsion outliers are listed below:

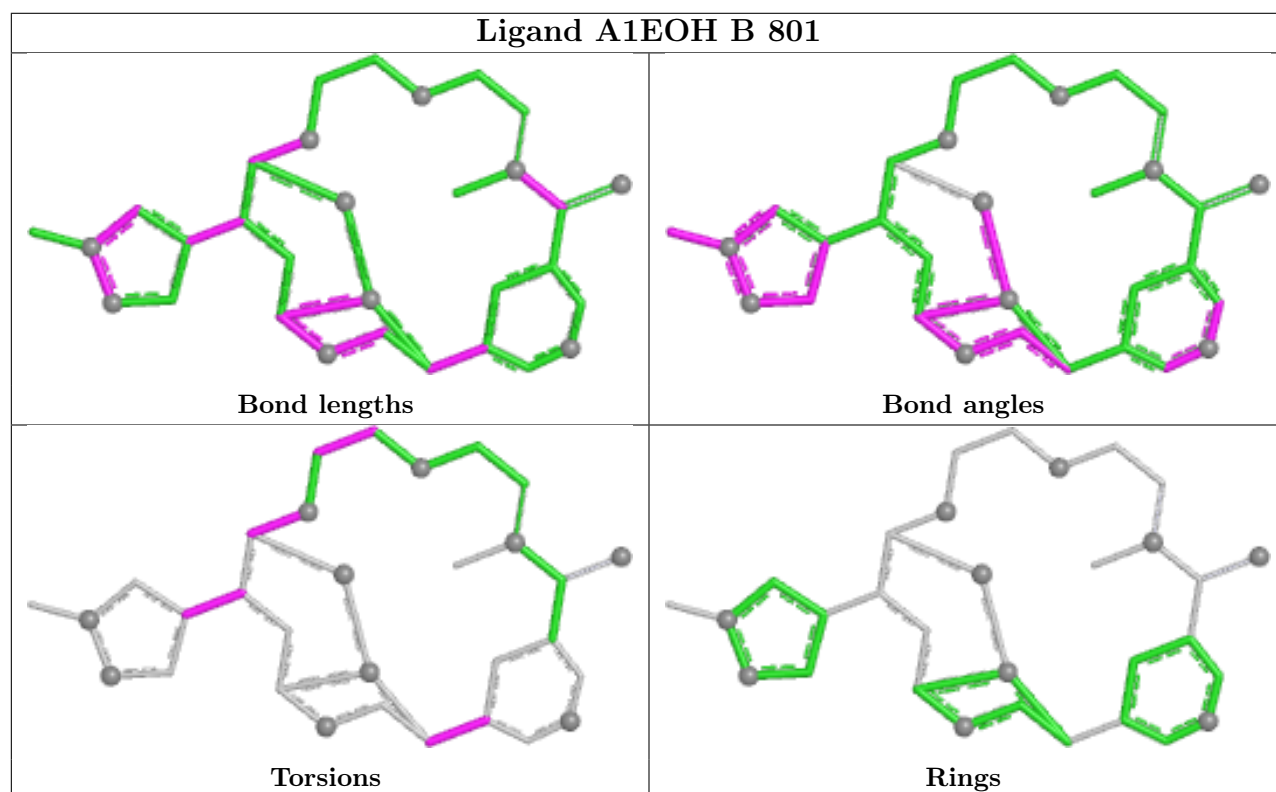
Mol	Chain	Res	Type	Atoms
2	A	801	A1EOH	C08-C07-C10-C23
2	A	801	A1EOH	N05-C07-C10-C23
2	A	801	A1EOH	C02-C03-O17-C18
2	A	801	A1EOH	N04-C03-O17-C18
2	B	801	A1EOH	C08-C07-C10-C23
2	B	801	A1EOH	N05-C07-C10-C23
2	B	801	A1EOH	C01-C02-C11-C12
2	B	801	A1EOH	O17-C18-C29-O30
2	A	801	A1EOH	O17-C18-C29-O30
2	A	801	A1EOH	N05-C07-C10-C19
2	B	801	A1EOH	N05-C07-C10-C19
2	B	801	A1EOH	C01-C02-C11-C15
2	B	801	A1EOH	C03-C02-C11-C15
2	A	801	A1EOH	C08-C07-C10-C19
2	B	801	A1EOH	C08-C07-C10-C19
2	B	801	A1EOH	N04-C03-O17-C18
2	A	801	A1EOH	C29-C18-O17-C03

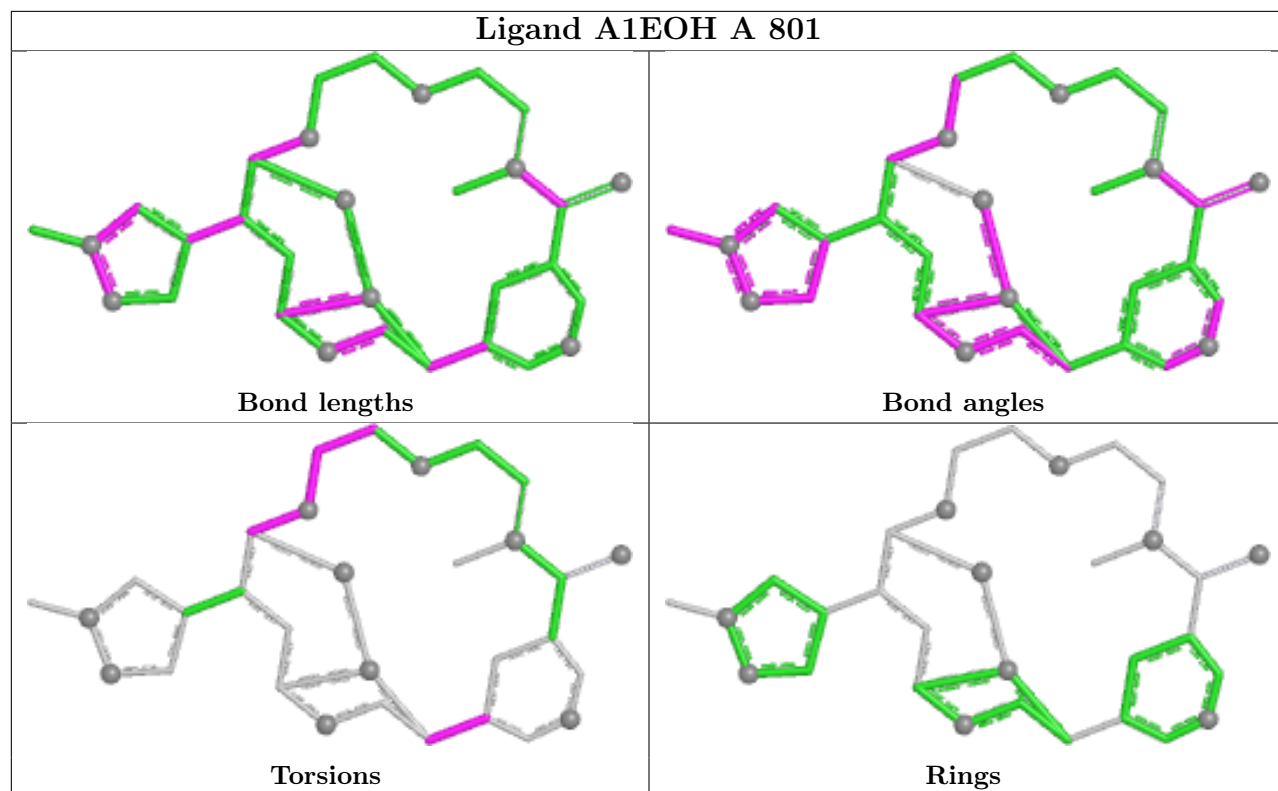
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	A1EOH	1	0
3	B	802	SO4	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	288/304 (94%)	1.25	45 (15%) 5 4	15, 29, 52, 77	1 (0%)
1	B	282/304 (92%)	1.16	38 (13%) 7 5	14, 28, 48, 71	1 (0%)
All	All	570/608 (93%)	1.21	83 (14%) 6 4	14, 28, 51, 77	2 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	491	CYS	6.8
1	B	654	ILE	6.0
1	A	653	ASN	5.7
1	A	657	TYR	5.2
1	B	594	PRO	4.9
1	B	595	GLU	4.8
1	A	542	GLY	4.8
1	A	654	ILE	4.6
1	B	467	GLU	4.5
1	B	652	ASN	4.5
1	A	763	LEU	4.5
1	B	542	GLY	4.3
1	A	594	PRO	4.3
1	A	593	VAL	4.2
1	B	651	ILE	4.1
1	B	593	VAL	3.9
1	B	541	ILE	3.9
1	B	653	ASN	3.6
1	A	727	ASN	3.6
1	A	656	TYR	3.6
1	A	726	ALA	3.5
1	A	660	THR	3.3
1	A	491	CYS	3.3
1	B	492	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	714	LYS	3.2
1	A	541	ILE	3.2
1	B	762	THR	3.2
1	A	595	GLU	3.2
1	A	581	PRO	3.1
1	B	592	ARG	3.0
1	A	644	ASP	2.9
1	B	540	MET	2.9
1	B	662	ASN	2.9
1	A	482	THR	2.8
1	B	650	ASP	2.8
1	B	493	GLY	2.8
1	A	598	MET	2.8
1	B	675	LEU	2.8
1	B	490	GLY	2.7
1	B	763	LEU	2.7
1	B	726	ALA	2.7
1	A	578	ALA	2.6
1	B	582	PRO	2.6
1	B	543	LYS	2.6
1	B	596	GLU	2.5
1	A	670	MET	2.5
1	A	632	VAL	2.5
1	A	490	GLY	2.5
1	B	495	VAL	2.5
1	A	467	GLU	2.4
1	B	632	VAL	2.4
1	A	580	ARG	2.4
1	A	651	ILE	2.4
1	B	603	LEU	2.4
1	A	489	GLU	2.4
1	B	663	GLY	2.3
1	B	578	ALA	2.3
1	A	745	SER	2.3
1	A	557	ASP	2.3
1	A	559	PRO	2.3
1	A	700	GLY	2.3
1	A	667	VAL	2.3
1	A	553	ALA	2.3
1	A	675	LEU	2.2
1	B	655	ASP	2.2
1	A	659	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	743	VAL	2.2
1	A	573	ARG	2.2
1	A	582	PRO	2.2
1	B	601	LYS	2.2
1	A	599	THR	2.2
1	B	581	PRO	2.1
1	B	481	LEU	2.1
1	B	743	VAL	2.1
1	A	628	ALA	2.1
1	A	699	LEU	2.1
1	B	599	THR	2.1
1	A	762	THR	2.0
1	A	571	ASN	2.0
1	A	627	LEU	2.0
1	A	696	ILE	2.0
1	A	501	VAL	2.0
1	B	487	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.

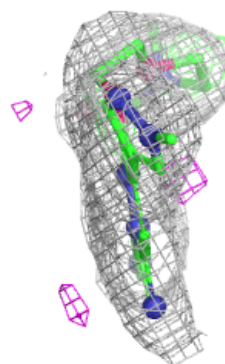
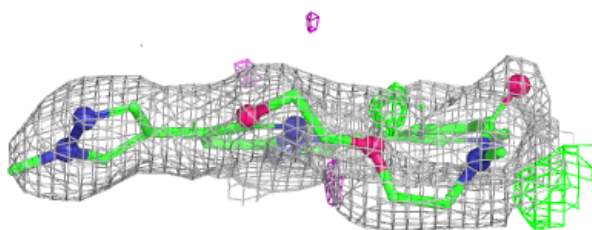
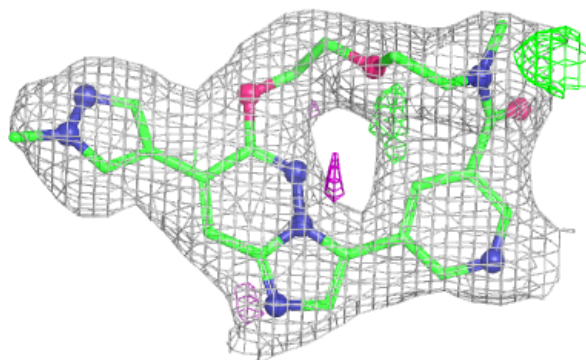
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	802	5/5	0.80	0.29	30,30,30,30	0
3	SO4	B	802	5/5	0.81	0.33	30,30,30,30	0
2	A1EOH	B	801	31/31	0.83	0.13	17,23,35,38	0
2	A1EOH	A	801	31/31	0.87	0.12	19,26,35,43	0

The following is a graphical depiction of the model fit to experimental electron density of all

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

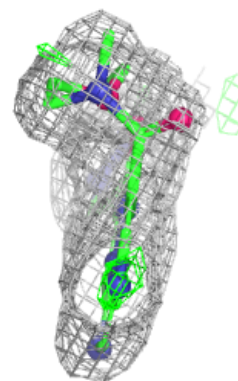
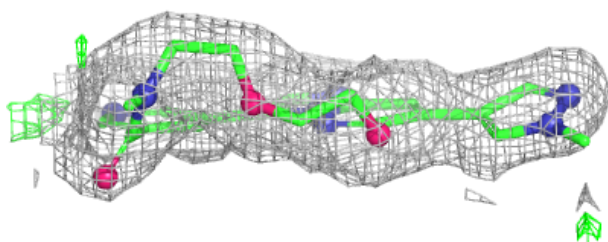
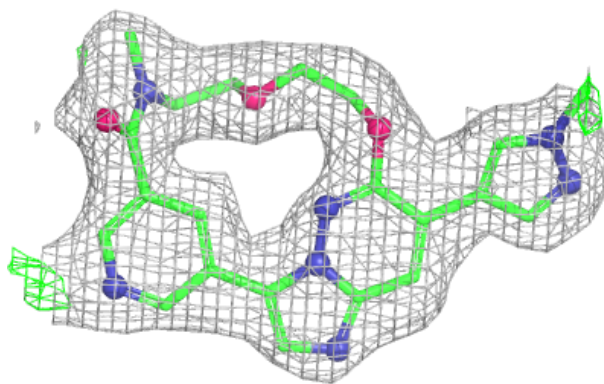
Electron density around A1EOH B 801:

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



Electron density around A1EOH A 801:

$2mF_o-DF_c$ (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.