



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2026 – 11:35 PM JST

PDB ID : 9W2L / pdb_00009w2l
Title : Crystal structure of FGFR2 with a macrocyclic compound XS9001
Authors : Chen, X.J.; Zhang, L.; Chen, Y.H.
Deposited on : 2025-07-28
Resolution : 2.10 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 : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

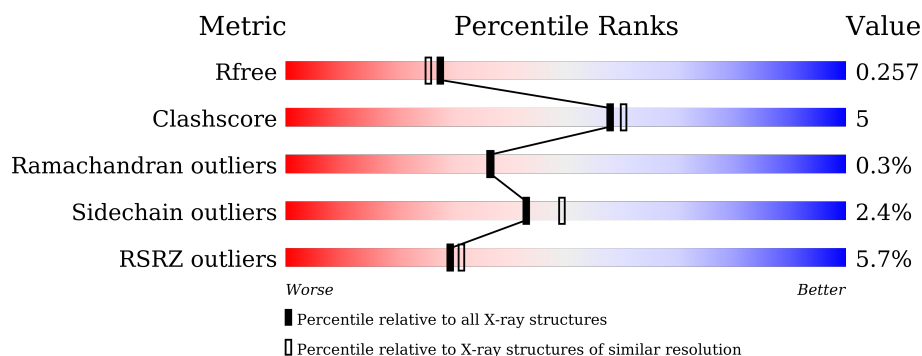
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	315	4% 86% 8% 5%
1	B	315	7% 80% 10% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	A1EVI	B	803	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5048 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.

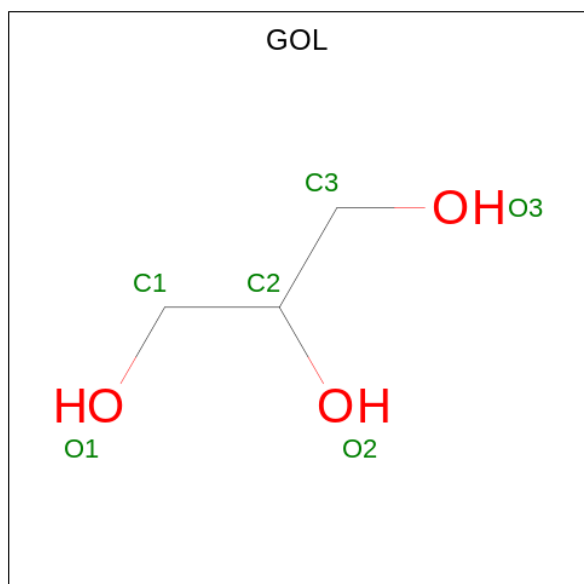
- Molecule 1 is a protein called Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	1	0
			2373	1511	398	441	23			
1	B	294	Total	C	N	O	S	0	1	0
			2343	1491	395	434	23			

There are 4 discrepancies between the modelled and reference sequences:

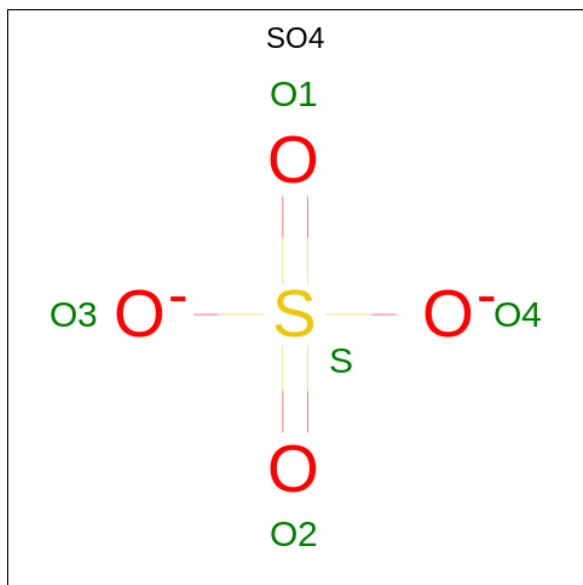
Chain	Residue	Modelled	Actual	Comment	Reference
A	454	GLY	-	expression tag	UNP P21802
A	455	PRO	-	expression tag	UNP P21802
B	454	GLY	-	expression tag	UNP P21802
B	455	PRO	-	expression tag	UNP P21802

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



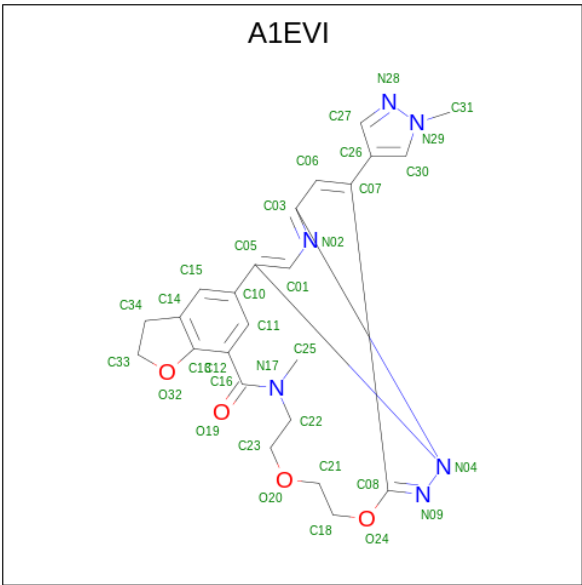
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- 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 XS9001 (CCD ID: A1EVI) (formula: C₂₄H₂₄N₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			34	24	6	4		
4	B	1	Total	C	N	O	0	0
			34	24	6	4		

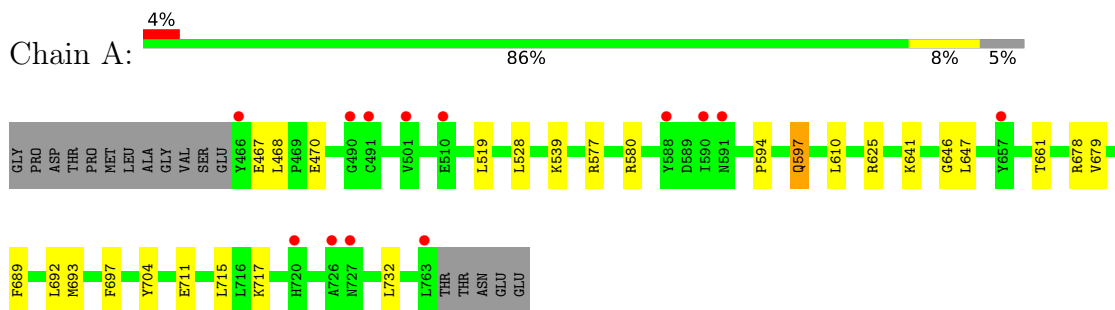
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	120	Total	O	0	0
			120	120		
5	B	122	Total	O	0	0
			122	122		

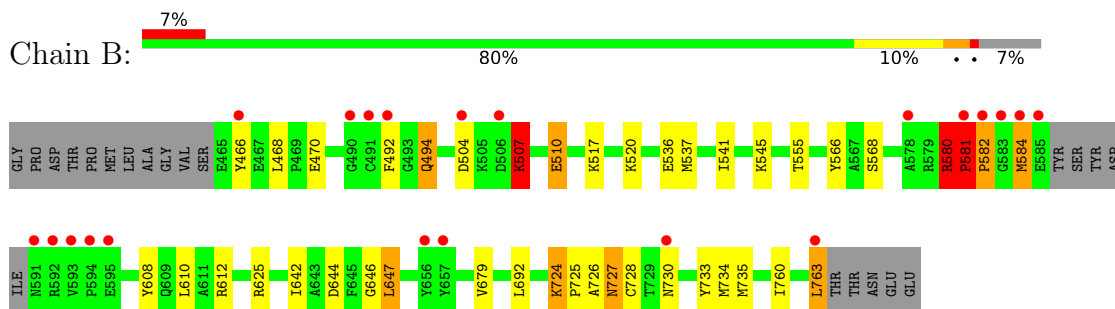
3 Residue-property plots [i](#)

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	60.91Å 72.57Å 137.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.34 – 2.10 16.34 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (16.34-2.10) 99.2 (16.34-2.10)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.228 , 0.260 0.226 , 0.257	Depositor DCC
R_{free} test set	1760 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5048	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 36.81 % 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 4.7230e-04. 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: A1EVI, SO4, GOL

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	0.43	2/2429 (0.1%)	0.39	0/3288
1	B	0.58	4/2396 (0.2%)	0.67	11/3239 (0.3%)
All	All	0.51	6/4825 (0.1%)	0.54	11/6527 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	704	TYR	C-O	-8.27	1.20	1.23
1	B	642	ILE	C-O	-6.71	1.16	1.24
1	B	644	ASP	C-O	-6.47	1.15	1.24
1	B	646	GLY	C-O	-5.82	1.16	1.23
1	B	647	LEU	C-O	-5.55	1.16	1.24
1	A	646	GLY	C-O	-5.38	1.17	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	581	PRO	N-CA-C	12.01	125.36	110.70
1	B	580	ARG	CA-C-N	10.69	131.39	120.38
1	B	580	ARG	C-N-CA	10.69	131.39	120.38
1	B	507	LYS	CA-C-N	6.85	127.72	120.12
1	B	507	LYS	C-N-CA	6.85	127.72	120.12
1	B	584	MET	N-CA-C	6.34	119.17	110.24
1	B	580	ARG	N-CA-C	-5.85	100.90	109.50
1	B	727	ASN	N-CA-C	5.50	122.51	110.80
1	B	724	LYS	CA-C-N	5.23	125.17	119.78
1	B	724	LYS	C-N-CA	5.23	125.17	119.78
1	B	504	ASP	N-CA-C	-5.17	100.31	108.73

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	2373	0	2342	15	0
1	B	2343	0	2329	30	0
2	A	6	0	8	1	0
2	B	6	0	8	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	34	0	0	0	0
4	B	34	0	0	0	0
5	A	120	0	0	2	0
5	B	122	0	0	0	0
All	All	5048	0	4687	43	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 (43) 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:581:PRO:HB2	1:B:582:PRO:HD3	1.55	0.87
1:B:760:ILE:HA	1:B:763:LEU:HD23	1.71	0.72
1:A:519:LEU:HD11	1:A:528:LEU:HD13	1.73	0.71
1:B:625:ARG:HH12	2:B:801:GOL:H32	1.61	0.65
1:B:545:LYS:CE	1:B:612:ARG:HH12	2.10	0.65
1:B:581:PRO:CB	1:B:582:PRO:HD3	2.28	0.64
1:B:724:LYS:CE	1:B:728:CYS:O	2.47	0.62
1:A:610:LEU:HD13	1:A:692:LEU:HD21	1.83	0.61
1:B:610:LEU:HD13	1:B:692:LEU:HD21	1.82	0.60
1:A:717:LYS:NZ	1:B:466:TYR:CE2	2.69	0.59
1:A:717:LYS:NZ	1:B:466:TYR:HE2	2.00	0.59
1:B:581:PRO:HB2	1:B:582:PRO:CD	2.31	0.58
1:B:625:ARG:HD3	1:B:647:LEU:O	2.04	0.58
1:A:641:LYS:NZ	5:A:908:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:LYS:HB3	2:A:801:GOL:H2	1.93	0.50
1:B:507:LYS:HB3	1:B:510:GLU:HG3	1.93	0.50
1:B:468:LEU:HD12	1:B:555:THR:HB	1.93	0.49
1:A:470:GLU:OE2	5:A:901:HOH:O	2.20	0.49
1:B:724:LYS:HE2	1:B:728:CYS:O	2.13	0.48
1:B:494:GLN:HB3	1:B:520:LYS:HG2	1.96	0.48
1:A:689:PHE:O	1:A:693:MET:HG3	2.14	0.47
1:A:661:THR:HB	1:A:678:ARG:HD2	1.97	0.47
1:A:625:ARG:HD3	1:A:647:LEU:O	2.16	0.46
1:A:711:GLU:O	1:A:715:LEU:HG	2.16	0.46
1:B:507:LYS:CB	1:B:510:GLU:HG3	2.46	0.45
1:B:726:ALA:O	1:B:727:ASN:OD1	2.35	0.45
1:A:577:ARG:O	1:A:580:ARG:HD3	2.17	0.45
1:B:536:GLU:OE2	1:B:536:GLU:HA	2.17	0.44
1:A:594:PRO:HA	1:A:597:GLN:CD	2.42	0.44
1:A:697:PHE:CZ	1:A:732:LEU:HD13	2.53	0.43
1:B:537:MET:HE2	1:B:537:MET:HB2	1.89	0.43
1:B:537:MET:O	1:B:541:ILE:HG23	2.19	0.43
1:B:580:ARG:HA	1:B:581:PRO:HD3	1.61	0.43
1:B:724:LYS:HG3	1:B:733:TYR:HB2	2.00	0.43
1:B:730:ASN:O	1:B:734:MET:HG2	2.19	0.43
1:B:492:PHE:O	1:B:517:LYS:HE3	2.20	0.42
1:B:566:TYR:CZ	1:B:568:SER:HA	2.55	0.41
1:B:724:LYS:HA	1:B:725:PRO:HD3	1.82	0.41
1:A:597:GLN:HA	1:A:597:GLN:OE1	2.21	0.41
1:B:545:LYS:NZ	1:B:612:ARG:HH12	2.18	0.41
1:B:608:TYR:HE2	1:B:612:ARG:HH21	1.68	0.41
1:B:545:LYS:HE3	1:B:612:ARG:HH12	1.86	0.40
1:B:735:MET:HE3	1:B:735:MET:HB2	1.97	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	297/315 (94%)	293 (99%)	4 (1%)	0	100	100
1	B	291/315 (92%)	283 (97%)	6 (2%)	2 (1%)	18	15
All	All	588/630 (93%)	576 (98%)	10 (2%)	2 (0%)	36	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	582	PRO
1	B	581	PRO

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	257/276 (93%)	253 (98%)	4 (2%)	55	64
1	B	255/276 (92%)	247 (97%)	8 (3%)	35	39
All	All	512/552 (93%)	500 (98%)	12 (2%)	43	51

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	467	GLU
1	A	468	LEU
1	A	597	GLN
1	A	679	VAL
1	B	470	GLU
1	B	494	GLN
1	B	507	LYS
1	B	510	GLU
1	B	580	ARG
1	B	584	MET
1	B	679	VAL
1	B	763	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	637	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	0.15	0	6,6,6	0.04	0
2	GOL	A	801	-	5,5,5	0.92	0	5,5,5	1.01	0
3	SO4	B	802	-	4,4,4	0.14	0	6,6,6	0.05	0
4	A1EVI	A	803	-	38,39,39	5.44	21 (55%)	48,57,57	10.61	27 (56%)
4	A1EVI	B	803	-	38,39,39	5.33	22 (57%)	48,57,57	10.34	24 (50%)
2	GOL	B	801	-	5,5,5	0.92	0	5,5,5	1.01	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
4	A1EVI	A	803	-	-	5/23/31/31	0/4/6/6
2	GOL	A	801	-	-	1/4/4/4	-
2	GOL	B	801	-	-	0/4/4/4	-
4	A1EVI	B	803	-	-	8/23/31/31	0/4/6/6

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	803	A1EVI	C01-C05	-16.18	1.22	1.37
4	A	803	A1EVI	C01-C05	-16.11	1.22	1.37
4	A	803	A1EVI	C13-C14	12.74	1.55	1.38
4	B	803	A1EVI	C13-C14	12.40	1.55	1.38
4	A	803	A1EVI	O32-C33	-11.73	1.24	1.45
4	B	803	A1EVI	O32-C33	-11.22	1.25	1.45
4	A	803	A1EVI	C03-N02	10.45	1.48	1.33
4	A	803	A1EVI	C15-C14	9.56	1.55	1.39
4	B	803	A1EVI	C05-N04	-9.29	1.24	1.38
4	B	803	A1EVI	C15-C14	9.07	1.55	1.39
4	A	803	A1EVI	C05-N04	-9.00	1.25	1.38
4	B	803	A1EVI	C03-N02	8.04	1.44	1.33
4	B	803	A1EVI	C12-C13	6.66	1.54	1.40
4	B	803	A1EVI	C34-C33	-6.43	1.35	1.52
4	A	803	A1EVI	C34-C33	-6.37	1.36	1.52
4	A	803	A1EVI	C11-C10	-6.24	1.30	1.39
4	B	803	A1EVI	C11-C10	-6.24	1.30	1.39
4	A	803	A1EVI	C12-C13	6.22	1.53	1.40
4	B	803	A1EVI	C15-C10	-5.46	1.31	1.39
4	A	803	A1EVI	C15-C10	-5.05	1.32	1.39
4	B	803	A1EVI	C11-C12	-4.84	1.32	1.39
4	B	803	A1EVI	C10-C05	4.52	1.55	1.48
4	A	803	A1EVI	C10-C05	4.39	1.55	1.48
4	B	803	A1EVI	C16-N17	4.29	1.41	1.34
4	A	803	A1EVI	C16-N17	4.13	1.41	1.34
4	A	803	A1EVI	O19-C16	-4.01	1.14	1.22
4	A	803	A1EVI	C30-C26	-3.78	1.33	1.38
4	B	803	A1EVI	O32-C13	3.62	1.43	1.38
4	A	803	A1EVI	C11-C12	-3.40	1.34	1.39
4	B	803	A1EVI	O19-C16	-3.30	1.16	1.22
4	A	803	A1EVI	C08-N09	3.23	1.33	1.28
4	A	803	A1EVI	O32-C13	3.22	1.42	1.38
4	B	803	A1EVI	C06-C03	-3.09	1.34	1.41
4	B	803	A1EVI	O24-C18	-3.07	1.36	1.45
4	A	803	A1EVI	C22-N17	-2.96	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	A1EVI	C31-N29	-2.91	1.42	1.46
4	B	803	A1EVI	C30-C26	-2.50	1.35	1.38
4	B	803	A1EVI	C31-N29	-2.44	1.43	1.46
4	A	803	A1EVI	O24-C18	-2.37	1.38	1.45
4	B	803	A1EVI	C22-N17	-2.35	1.42	1.47
4	B	803	A1EVI	C12-C16	2.31	1.54	1.50
4	A	803	A1EVI	C06-C03	-2.31	1.36	1.41
4	B	803	A1EVI	C08-N09	2.17	1.31	1.28

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	A1EVI	C01-C05-N04	64.71	119.37	103.47
4	B	803	A1EVI	C01-C05-N04	63.63	119.11	103.47
4	A	803	A1EVI	O32-C33-C34	16.32	125.46	107.92
4	B	803	A1EVI	O32-C33-C34	15.88	124.99	107.92
4	B	803	A1EVI	O32-C13-C14	-11.95	105.77	113.59
4	A	803	A1EVI	O32-C13-C14	-10.05	107.01	113.59
4	B	803	A1EVI	C10-C05-C01	-9.93	115.36	129.81
4	A	803	A1EVI	C01-N02-C03	-9.76	100.57	105.11
4	A	803	A1EVI	C10-C05-C01	-9.48	116.01	129.81
4	A	803	A1EVI	C34-C14-C15	9.38	144.72	129.41
4	A	803	A1EVI	C31-N29-N28	9.28	126.47	120.24
4	A	803	A1EVI	C15-C14-C13	-9.27	112.61	120.14
4	B	803	A1EVI	C15-C14-C13	-9.24	112.64	120.14
4	A	803	A1EVI	C33-O32-C13	-8.86	100.71	107.04
4	B	803	A1EVI	C34-C14-C15	8.49	143.26	129.41
4	A	803	A1EVI	C34-C14-C13	-7.81	102.67	107.98
4	B	803	A1EVI	C01-N02-C03	-7.54	101.60	105.11
4	B	803	A1EVI	C31-N29-N28	7.51	125.28	120.24
4	B	803	A1EVI	C27-N28-N29	6.74	108.08	104.36
4	A	803	A1EVI	C33-C34-C14	-6.64	96.36	102.02
4	B	803	A1EVI	C30-N29-N28	-6.31	108.79	112.09
4	B	803	A1EVI	O32-C13-C12	5.91	141.69	126.72
4	B	803	A1EVI	C34-C14-C13	-5.72	104.09	107.98
4	A	803	A1EVI	O32-C13-C12	5.62	140.97	126.72
4	A	803	A1EVI	C13-C12-C16	-5.15	109.08	124.29
4	B	803	A1EVI	O19-C16-N17	-4.42	117.08	122.41
4	A	803	A1EVI	C11-C12-C13	4.21	125.36	119.04
4	A	803	A1EVI	C30-N29-N28	-4.14	109.92	112.09
4	B	803	A1EVI	C26-C27-N28	-4.14	108.91	112.14
4	A	803	A1EVI	C31-N29-C30	-4.13	123.60	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	A1EVI	C13-C12-C16	-3.99	112.49	124.29
4	B	803	A1EVI	C03-N04-N09	-3.79	123.21	126.88
4	A	803	A1EVI	C03-N04-N09	-3.66	123.33	126.88
4	B	803	A1EVI	C11-C12-C13	3.59	124.43	119.04
4	A	803	A1EVI	C26-C27-N28	-3.50	109.41	112.14
4	A	803	A1EVI	O19-C16-N17	-3.42	118.29	122.41
4	A	803	A1EVI	C06-C03-N02	3.28	135.50	129.99
4	B	803	A1EVI	C33-C34-C14	-3.25	99.25	102.02
4	B	803	A1EVI	C33-O32-C13	-3.10	104.83	107.04
4	B	803	A1EVI	C11-C10-C15	2.92	123.15	119.63
4	A	803	A1EVI	C15-C10-C05	-2.87	114.73	120.67
4	A	803	A1EVI	C27-N28-N29	2.83	105.92	104.36
4	B	803	A1EVI	C05-C01-N02	-2.82	108.59	111.99
4	B	803	A1EVI	C15-C10-C05	-2.64	115.20	120.67
4	A	803	A1EVI	C23-C22-N17	-2.52	106.28	112.29
4	B	803	A1EVI	C06-C03-N02	2.49	134.17	129.99
4	B	803	A1EVI	C25-N17-C22	2.48	120.91	115.89
4	A	803	A1EVI	C10-C15-C14	2.36	125.07	121.47
4	A	803	A1EVI	C11-C12-C16	2.35	125.55	118.58
4	A	803	A1EVI	C30-C26-C27	2.21	106.05	104.05
4	A	803	A1EVI	C11-C10-C15	2.11	122.18	119.63

There are no chirality outliers.

All (14) torsion outliers are listed below:

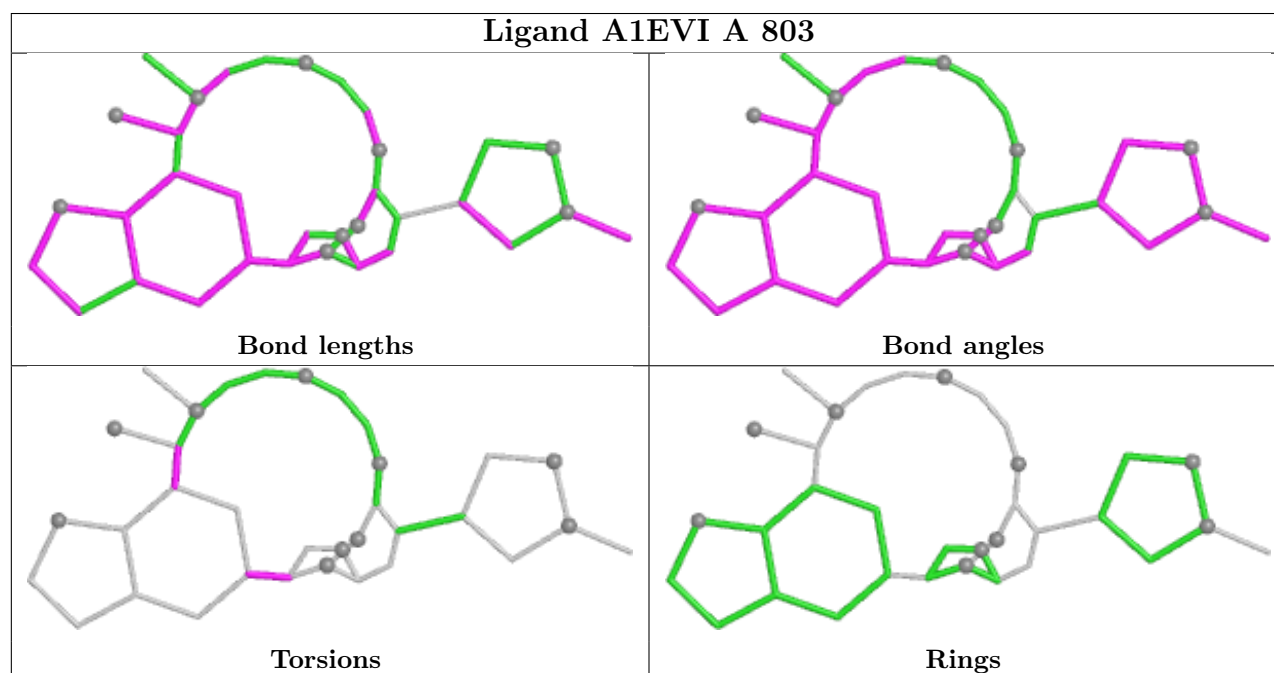
Mol	Chain	Res	Type	Atoms
4	A	803	A1EVI	N04-C05-C10-C15
4	B	803	A1EVI	N04-C05-C10-C15
4	B	803	A1EVI	O24-C18-C21-O20
4	A	803	A1EVI	N04-C05-C10-C11
4	B	803	A1EVI	N04-C05-C10-C11
4	B	803	A1EVI	N17-C22-C23-O20
2	A	801	GOL	O1-C1-C2-O2
4	B	803	A1EVI	C01-C05-C10-C15
4	A	803	A1EVI	C01-C05-C10-C15
4	A	803	A1EVI	C01-C05-C10-C11
4	B	803	A1EVI	C01-C05-C10-C11
4	A	803	A1EVI	C13-C12-C16-O19
4	B	803	A1EVI	C13-C12-C16-O19
4	B	803	A1EVI	C18-C21-O20-C23

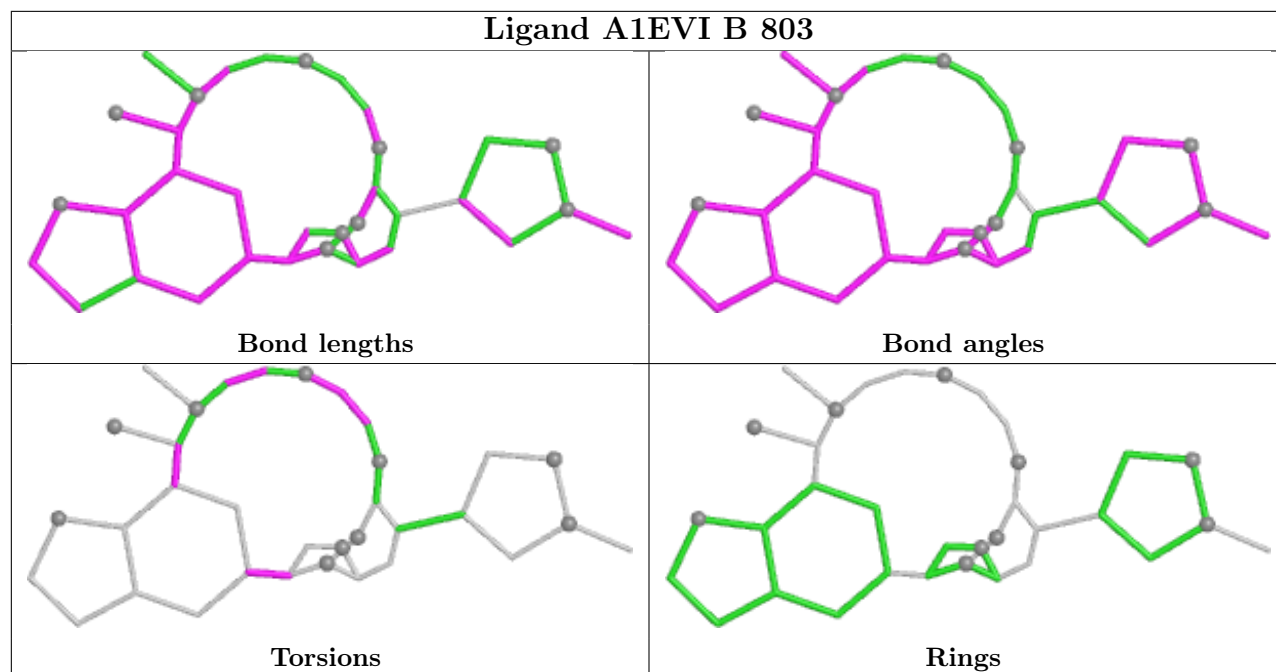
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	GOL	1	0
2	B	801	GOL	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	298/315 (94%)	0.43	13 (4%) 39 41	17, 27, 51, 69	1 (0%)
1	B	294/315 (93%)	0.40	21 (7%) 22 23	16, 27, 61, 84	1 (0%)
All	All	592/630 (93%)	0.42	34 (5%) 29 31	16, 27, 57, 84	2 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	466	TYR	5.0
1	B	584	MET	4.8
1	B	594	PRO	4.4
1	B	492	PHE	4.2
1	A	763	LEU	3.9
1	A	466	TYR	3.7
1	A	491	CYS	3.6
1	A	510	GLU	3.3
1	A	727	ASN	3.1
1	B	583	GLY	3.1
1	B	582	PRO	3.0
1	A	591	ASN	3.0
1	B	593	VAL	2.9
1	B	581	PRO	2.9
1	B	490	GLY	2.9
1	B	491	CYS	2.9
1	B	591	ASN	2.8
1	A	590	ILE	2.7
1	A	720	HIS	2.6
1	A	490	GLY	2.6
1	B	595	GLU	2.5
1	B	506	ASP	2.5
1	B	585	GLU	2.5
1	B	578	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	726	ALA	2.3
1	B	763	LEU	2.3
1	A	657	TYR	2.3
1	B	656	TYR	2.3
1	B	657	TYR	2.3
1	B	592	ARG	2.3
1	A	588	TYR	2.3
1	B	730	ASN	2.2
1	B	504	ASP	2.1
1	A	501	VAL	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](#)

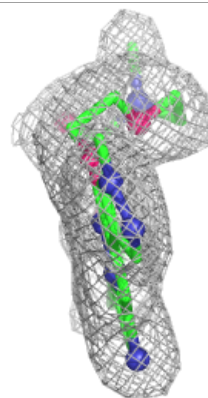
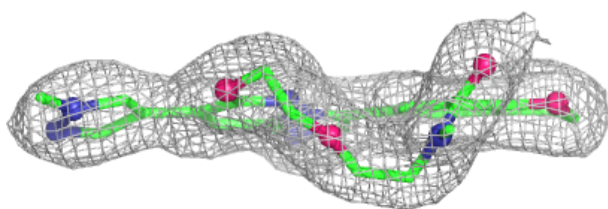
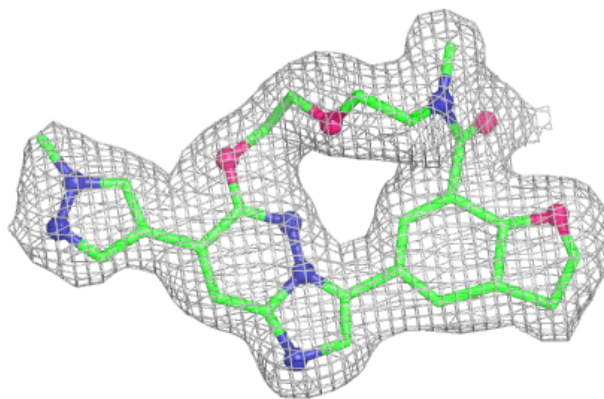
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	802	5/5	0.72	0.20	37,38,50,56	0
2	GOL	B	801	6/6	0.83	0.12	22,29,35,39	0
2	GOL	A	801	6/6	0.85	0.12	28,33,37,39	0
3	SO4	B	802	5/5	0.85	0.13	43,47,66,66	0
4	A1EVI	A	803	34/34	0.93	0.07	22,29,34,39	0
4	A1EVI	B	803	34/34	0.94	0.07	22,28,34,41	0

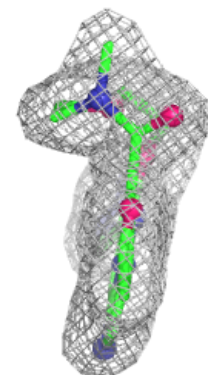
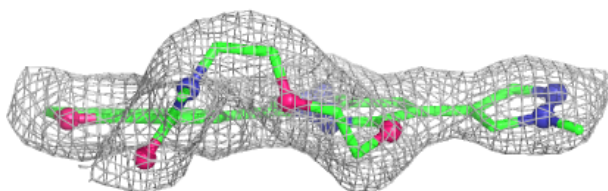
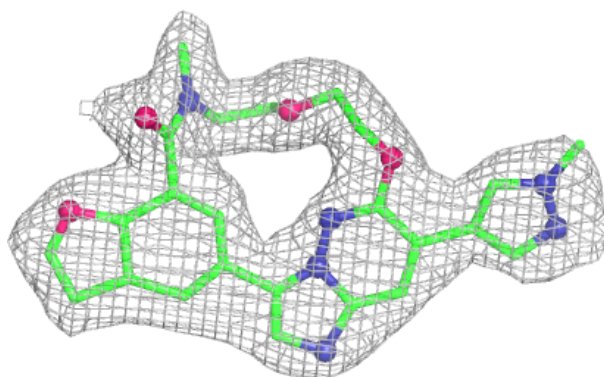
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1EVI A 803:

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

**Electron density around A1EVI B 803:**

$2mF_o-DF_c$ (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.