



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2026 – 02:08 PM JST

PDB ID : 9VLM / pdb_00009vlm
Title : The X-RAY co-crystal structure of human FGFR2 and covalent inhibitor 10a
Authors : Chen, X.J.; Liu, X.R.; Zhang, L.; Chen, Y.H.
Deposited on : 2025-06-25
Resolution : 2.26 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 : 9.0.010 (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

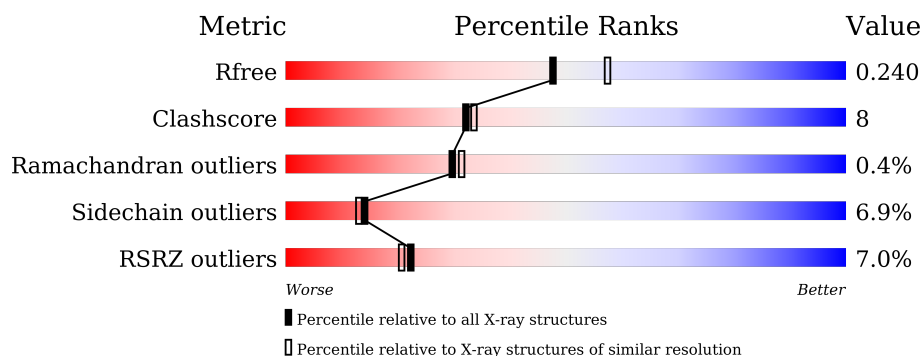
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	303	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>• 8%</div> </div> </div>
1	B	303	<div> <div>9%</div> <div> <div></div> <div>72%</div> <div>17%</div> <div>• • 8%</div> </div> </div>

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
3	GOL	A	802	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4616 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.

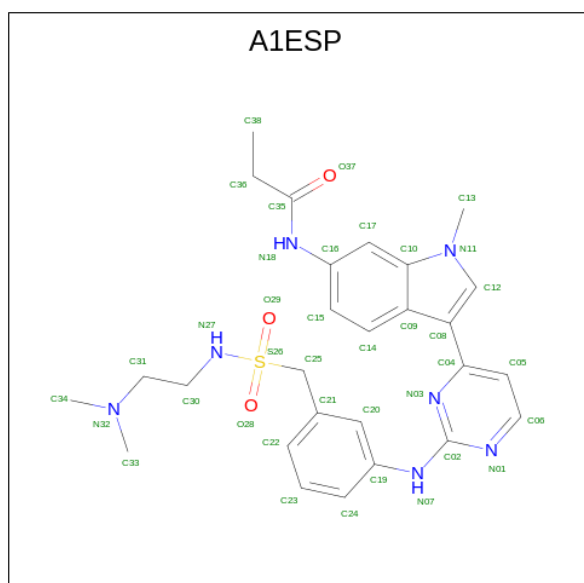
- Molecule 1 is a protein called Fibroblast growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2202	1402	370	409	21			
1	B	280	Total	C	N	O	S	0	0	0
			2204	1404	368	410	22			

There are 4 discrepancies between the modelled and reference sequences:

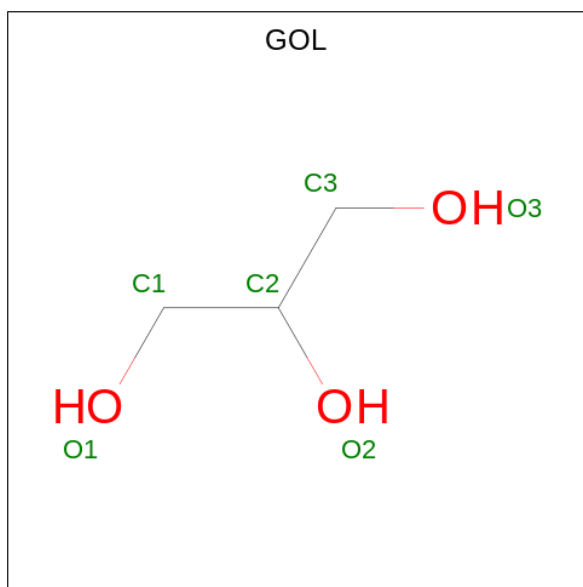
Chain	Residue	Modelled	Actual	Comment	Reference
A	463	GLY	-	expression tag	UNP P21802
A	464	PRO	-	expression tag	UNP P21802
B	463	GLY	-	expression tag	UNP P21802
B	464	PRO	-	expression tag	UNP P21802

- Molecule 2 is {N}-[3-[2-[[3-[2-(dimethylamino)ethylsulfamoylmethyl]phenyl]amino]pyrimidin-4-yl]-1-methyl-indol-6-yl]propanamide (CCD ID: A1ESP) (formula: C₂₇H₃₃N₇O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			38	27	7	3	1		
2	B	1	Total	C	N	O	S	0	0
			38	27	7	3	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

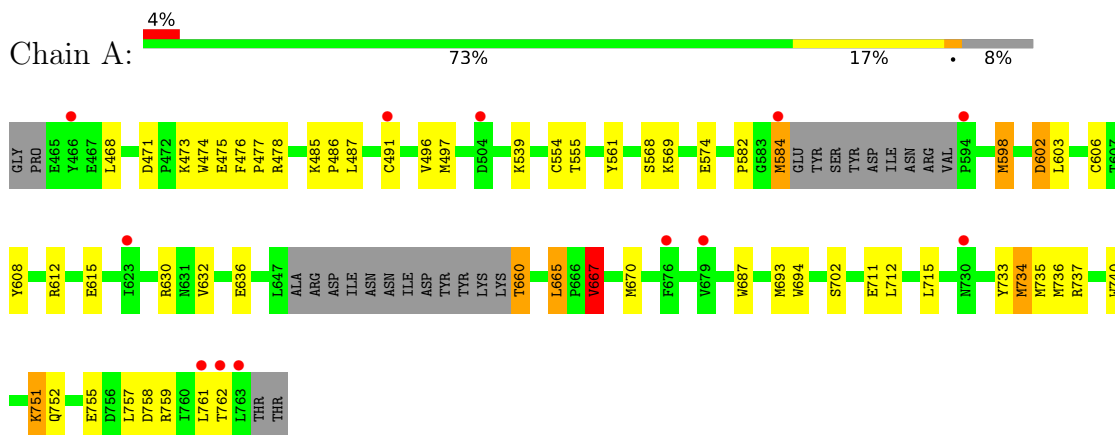
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	60	Total	O	0	0
			60	60		

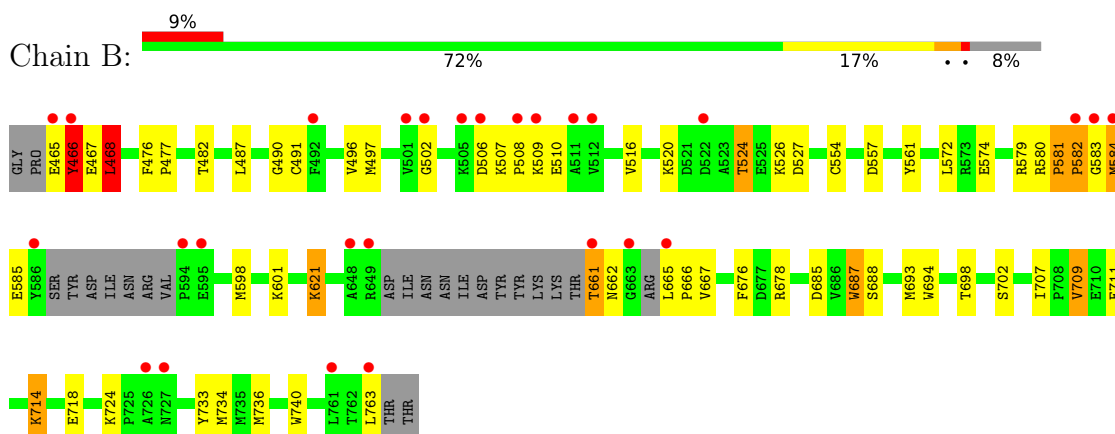
3 Residue-property plots [i](#)

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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.98Å 47.56Å 108.90Å 90.00° 101.57° 90.00°	Depositor
Resolution (Å)	53.34 – 2.26 53.34 – 2.26	Depositor EDS
% Data completeness (in resolution range)	96.5 (53.34-2.26) 96.5 (53.34-2.26)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.27Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.207 , 0.254 0.206 , 0.240	Depositor DCC
R_{free} test set	1363 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4616	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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: A1ESP, 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	1.07	7/2249 (0.3%)	0.84	11/3040 (0.4%)
1	B	1.04	5/2250 (0.2%)	0.88	14/3041 (0.5%)
All	All	1.06	12/4499 (0.3%)	0.86	25/6081 (0.4%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	490	GLY	C-N	-7.54	1.23	1.33
1	A	602	ASP	C-O	-6.13	1.17	1.24
1	A	632	VAL	C-O	-5.83	1.17	1.24
1	B	688	SER	C-O	-5.58	1.17	1.24
1	B	676	PHE	C-O	-5.42	1.17	1.24
1	B	687	TRP	C-O	-5.42	1.17	1.24
1	A	665	LEU	C-O	-5.40	1.19	1.24
1	A	598	MET	C-O	-5.22	1.17	1.24
1	A	603	LEU	C-O	-5.18	1.18	1.24
1	A	693	MET	C-O	-5.18	1.18	1.24
1	A	734	MET	C-O	-5.10	1.18	1.24
1	B	685	ASP	C-O	-5.09	1.17	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	665	LEU	CA-C-N	9.44	130.08	119.32
1	A	665	LEU	C-N-CA	9.44	130.08	119.32
1	B	667	VAL	N-CA-C	8.55	119.34	110.36
1	B	466	TYR	N-CA-C	8.26	121.96	109.41
1	A	471	ASP	CA-C-N	7.62	129.37	119.84
1	A	471	ASP	C-N-CA	7.62	129.37	119.84
1	B	468	LEU	CA-C-N	7.01	127.40	119.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	468	LEU	C-N-CA	7.01	127.40	119.83
1	A	485	LYS	CA-C-N	6.86	126.62	119.76
1	A	485	LYS	C-N-CA	6.86	126.62	119.76
1	B	491	CYS	O-C-N	6.61	129.23	122.09
1	A	712	LEU	N-CA-C	6.00	118.31	111.11
1	B	583	GLY	N-CA-C	5.92	122.03	111.01
1	B	678	ARG	N-CA-C	5.87	119.49	111.39
1	A	491	CYS	O-C-N	5.67	129.04	122.17
1	A	568	SER	N-CA-C	5.66	119.28	112.38
1	B	580	ARG	N-CA-C	-5.63	102.56	109.65
1	A	667	VAL	CB-CA-C	-5.56	104.75	112.04
1	A	582	PRO	N-CA-C	5.46	119.19	110.40
1	B	707	ILE	N-CA-C	5.42	113.84	107.77
1	B	584	MET	N-CA-C	-5.24	106.75	112.72
1	B	506	ASP	CA-C-N	-5.23	117.03	122.89
1	B	506	ASP	C-N-CA	-5.23	117.03	122.89
1	B	572	LEU	N-CA-C	5.08	116.82	111.28
1	B	709	VAL	N-CA-C	5.06	117.37	111.05

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	2202	0	2182	37	0
1	B	2204	0	2170	36	0
2	A	38	0	0	0	0
2	B	38	0	0	0	0
3	A	6	0	8	9	0
3	B	6	0	8	0	0
4	A	62	0	0	0	0
4	B	60	0	0	0	0
All	All	4616	0	4368	71	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 8.

All (71) 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:CD	1.60	1.29
1:B:581:PRO:CB	1:B:582:PRO:HD3	1.49	1.21
1:A:584:MET:HB2	1:B:661:THR:N	1.74	1.02
1:B:581:PRO:HB2	1:B:582:PRO:HD3	1.04	1.01
1:A:630:ARG:HH12	3:A:802:GOL:H32	1.32	0.93
1:B:665:LEU:HB3	1:B:666:PRO:HD3	1.51	0.91
1:A:630:ARG:HH22	3:A:802:GOL:H31	1.32	0.91
1:B:581:PRO:HB3	1:B:582:PRO:HD3	1.53	0.90
1:B:581:PRO:CB	1:B:582:PRO:CD	2.29	0.86
1:B:507:LYS:CB	1:B:510:GLU:HB3	2.15	0.77
1:A:630:ARG:NH1	3:A:802:GOL:H32	2.03	0.74
1:A:630:ARG:HH22	3:A:802:GOL:C3	2.04	0.70
1:A:694:TRP:HD1	1:A:736:MET:HE1	1.57	0.70
1:B:665:LEU:HB3	1:B:666:PRO:CD	2.24	0.68
1:A:554:CYS:HB2	1:A:561:TYR:HB2	1.77	0.65
1:B:579:ARG:HH11	1:B:579:ARG:HG3	1.62	0.65
1:B:581:PRO:HB2	1:B:582:PRO:HD2	1.70	0.65
1:B:662:ASN:HB3	1:B:665:LEU:HG	1.78	0.65
1:A:630:ARG:HH12	3:A:802:GOL:C3	2.07	0.62
1:B:466:TYR:HD2	1:B:468:LEU:HD21	1.65	0.61
1:B:524:THR:HG22	1:B:527:ASP:H	1.66	0.60
1:B:487:LEU:HD21	1:B:497:MET:HE2	1.86	0.58
1:B:574:GLU:OE2	1:B:574:GLU:HA	2.03	0.58
1:B:724:LYS:HG3	1:B:733:TYR:HB2	1.86	0.58
1:A:630:ARG:HH12	3:A:802:GOL:H12	1.69	0.57
1:A:584:MET:CB	1:B:661:THR:N	2.59	0.57
1:A:660:THR:HG22	1:A:665:LEU:HD21	1.87	0.57
1:B:468:LEU:HD22	1:B:468:LEU:N	2.20	0.56
1:B:554:CYS:HB2	1:B:561:TYR:HB2	1.89	0.55
1:A:733:TYR:CZ	1:A:737:ARG:HD3	2.43	0.53
1:A:474:TRP:CD1	1:A:539:LYS:HD3	2.44	0.53
1:A:475:GLU:OE1	1:A:555:THR:OG1	2.25	0.52
1:A:755:GLU:HG2	1:A:759:ARG:HH21	1.76	0.51
1:A:757:LEU:O	1:A:761:LEU:HD23	2.11	0.50
1:A:584:MET:C	1:A:584:MET:HE3	2.37	0.50
1:A:486:PRO:HA	1:A:496:VAL:HG12	1.93	0.50
1:A:630:ARG:NH1	3:A:802:GOL:H12	2.26	0.50
1:B:714:LYS:O	1:B:718:GLU:HG3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:TRP:O	1:B:698:THR:HG23	2.11	0.49
1:A:474:TRP:NE1	1:A:539:LYS:HD3	2.27	0.49
1:A:687:TRP:CE3	1:A:740:TRP:HA	2.48	0.49
1:B:621:LYS:HA	1:B:621:LYS:HD2	1.49	0.48
1:B:693:MET:HE2	1:B:736:MET:HG3	1.96	0.48
1:B:661:THR:HB	1:B:662:ASN:HD22	1.77	0.48
1:A:694:TRP:HB2	1:A:736:MET:HE3	1.96	0.48
1:A:667:VAL:HA	1:A:670:MET:SD	2.55	0.47
1:B:665:LEU:HD12	1:B:665:LEU:HA	1.80	0.47
1:B:502:GLY:HA2	1:B:508:PRO:HA	1.96	0.46
1:A:615:GLU:HG3	1:A:751:LYS:HE3	1.98	0.46
1:B:466:TYR:CD1	1:B:466:TYR:N	2.85	0.45
1:A:660:THR:CG2	1:A:665:LEU:HD21	2.45	0.45
1:B:476:PHE:HA	1:B:477:PRO:HD3	1.82	0.45
1:A:487:LEU:HD21	1:A:497:MET:HE2	1.99	0.45
1:A:736:MET:HE3	1:A:740:TRP:CH2	2.52	0.44
1:B:687:TRP:CE3	1:B:740:TRP:HA	2.53	0.44
1:A:660:THR:O	1:A:660:THR:OG1	2.33	0.44
1:B:465:GLU:HG2	1:B:466:TYR:HD1	1.82	0.44
1:A:615:GLU:CG	1:A:751:LYS:HE3	2.48	0.43
1:B:468:LEU:HD22	1:B:468:LEU:H	1.82	0.43
1:A:598:MET:HE3	1:A:602:ASP:HB3	2.00	0.43
1:A:711:GLU:O	1:A:715:LEU:HD12	2.18	0.43
1:B:579:ARG:HH11	1:B:579:ARG:CG	2.30	0.43
1:B:598:MET:HE3	1:B:598:MET:HB3	1.95	0.42
1:A:608:TYR:CZ	1:A:612:ARG:HD2	2.55	0.42
1:A:630:ARG:HH12	3:A:802:GOL:C1	2.33	0.42
1:B:687:TRP:CD1	1:B:687:TRP:C	2.97	0.42
1:A:630:ARG:NH2	3:A:802:GOL:C3	2.79	0.42
1:A:758:ASP:O	1:A:762:THR:HB	2.20	0.41
1:A:569:LYS:NZ	1:A:636:GLU:O	2.54	0.41
1:A:476:PHE:HA	1:A:477:PRO:HD3	1.95	0.41
1:B:496:VAL:HG22	1:B:516:VAL:HG22	2.02	0.41

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	272/303 (90%)	270 (99%)	2 (1%)	0	100	100
1	B	272/303 (90%)	266 (98%)	4 (2%)	2 (1%)	18	17
All	All	544/606 (90%)	536 (98%)	6 (1%)	2 (0%)	30	31

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	239/266 (90%)	226 (95%)	13 (5%)	20	21
1	B	237/266 (89%)	217 (92%)	20 (8%)	10	8
All	All	476/532 (90%)	443 (93%)	33 (7%)	14	13

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	468	LEU
1	A	473	LYS
1	A	478	ARG
1	A	574	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	584	MET
1	A	606	CYS
1	A	660	THR
1	A	667	VAL
1	A	702	SER
1	A	734	MET
1	A	735	MET
1	A	751	LYS
1	A	752	GLN
1	B	466	TYR
1	B	467	GLU
1	B	468	LEU
1	B	482	THR
1	B	509	LYS
1	B	520	LYS
1	B	524	THR
1	B	526	LYS
1	B	557	ASP
1	B	584	MET
1	B	585	GLU
1	B	601	LYS
1	B	621	LYS
1	B	661	THR
1	B	702	SER
1	B	709	VAL
1	B	711	GLU
1	B	714	LYS
1	B	734	MET
1	B	763	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	730	ASN
1	A	752	GLN
1	B	662	ASN
1	B	720	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	GOL	A	802	-	5,5,5	0.43	0	5,5,5	0.38	0
2	A1ESP	B	801	1	39,41,41	1.83	11 (28%)	56,58,58	2.59	9 (16%)
3	GOL	B	802	-	5,5,5	0.90	0	5,5,5	1.00	0
2	A1ESP	A	801	1	39,41,41	1.81	11 (28%)	56,58,58	2.63	14 (25%)

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	GOL	A	802	-	-	0/4/4/4	-
2	A1ESP	B	801	1	-	10/26/26/26	0/4/4/4
3	GOL	B	802	-	-	0/4/4/4	-
2	A1ESP	A	801	1	-	6/26/26/26	0/4/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	A1ESP	C02-N07	4.93	1.46	1.36
2	A	801	A1ESP	C02-N07	4.79	1.46	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	A1ESP	C35-N18	4.78	1.46	1.35
2	B	801	A1ESP	C35-N18	4.76	1.46	1.35
2	B	801	A1ESP	S26-N27	4.09	1.71	1.61
2	A	801	A1ESP	S26-N27	3.89	1.71	1.61
2	A	801	A1ESP	C12-N11	-2.80	1.32	1.37
2	B	801	A1ESP	C12-N11	-2.77	1.32	1.37
2	B	801	A1ESP	C19-N07	2.62	1.46	1.40
2	A	801	A1ESP	C09-C10	-2.57	1.37	1.41
2	B	801	A1ESP	C09-C10	-2.55	1.37	1.41
2	A	801	A1ESP	C19-N07	2.54	1.46	1.40
2	B	801	A1ESP	O28-S26	2.36	1.46	1.43
2	A	801	A1ESP	O28-S26	2.32	1.46	1.43
2	B	801	A1ESP	O29-S26	2.28	1.46	1.43
2	A	801	A1ESP	O29-S26	2.27	1.46	1.43
2	A	801	A1ESP	C16-N18	2.26	1.46	1.41
2	B	801	A1ESP	C16-N18	2.18	1.46	1.41
2	B	801	A1ESP	C12-C08	2.18	1.39	1.37
2	B	801	A1ESP	O37-C35	-2.10	1.19	1.23
2	A	801	A1ESP	C12-C08	2.09	1.39	1.37
2	A	801	A1ESP	O37-C35	-2.08	1.19	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	A1ESP	O29-S26-O28	-13.25	100.16	119.35
2	A	801	A1ESP	O29-S26-O28	-12.93	100.62	119.35
2	A	801	A1ESP	C06-N01-C02	7.61	122.20	115.45
2	B	801	A1ESP	C06-N01-C02	7.35	121.97	115.45
2	B	801	A1ESP	N01-C02-N03	-5.75	121.10	126.55
2	A	801	A1ESP	N01-C02-N03	-5.51	121.32	126.55
2	A	801	A1ESP	C05-C06-N01	-4.79	118.01	123.96
2	B	801	A1ESP	C04-N03-C02	4.70	120.60	116.80
2	B	801	A1ESP	C05-C06-N01	-4.56	118.30	123.96
2	B	801	A1ESP	C08-C12-N11	-4.40	109.68	111.05
2	A	801	A1ESP	C08-C12-N11	-4.10	109.78	111.05
2	A	801	A1ESP	C04-N03-C02	4.05	120.07	116.80
2	A	801	A1ESP	O28-S26-C25	3.45	113.56	108.30
2	B	801	A1ESP	C05-C04-N03	-2.59	119.89	122.92
2	A	801	A1ESP	C05-C04-N03	-2.48	120.01	122.92
2	A	801	A1ESP	C21-C25-S26	2.46	117.59	112.34
2	B	801	A1ESP	O28-S26-N27	2.42	112.47	106.97
2	A	801	A1ESP	C25-C21-C22	2.32	123.43	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	A1ESP	C06-C05-C04	2.23	118.38	117.02
2	A	801	A1ESP	O28-S26-N27	2.21	112.00	106.97
2	A	801	A1ESP	C10-N11-C12	2.14	110.09	108.54
2	A	801	A1ESP	C09-C08-C12	-2.11	104.76	106.00
2	B	801	A1ESP	C10-N11-C12	2.09	110.06	108.54

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	A1ESP	C20-C21-C25-S26
2	A	801	A1ESP	C22-C21-C25-S26
2	A	801	A1ESP	C21-C25-S26-O29
2	A	801	A1ESP	N27-C30-C31-N32
2	A	801	A1ESP	C30-N27-S26-O28
2	B	801	A1ESP	C21-C25-S26-N27
2	B	801	A1ESP	C21-C25-S26-O28
2	B	801	A1ESP	C21-C25-S26-O29
2	B	801	A1ESP	C30-N27-S26-C25
2	B	801	A1ESP	C30-N27-S26-O28
2	B	801	A1ESP	C30-N27-S26-O29
2	B	801	A1ESP	C30-C31-N32-C33
2	A	801	A1ESP	N03-C04-C08-C09
2	B	801	A1ESP	N03-C04-C08-C09
2	B	801	A1ESP	C31-C30-N27-S26
2	B	801	A1ESP	N27-C30-C31-N32

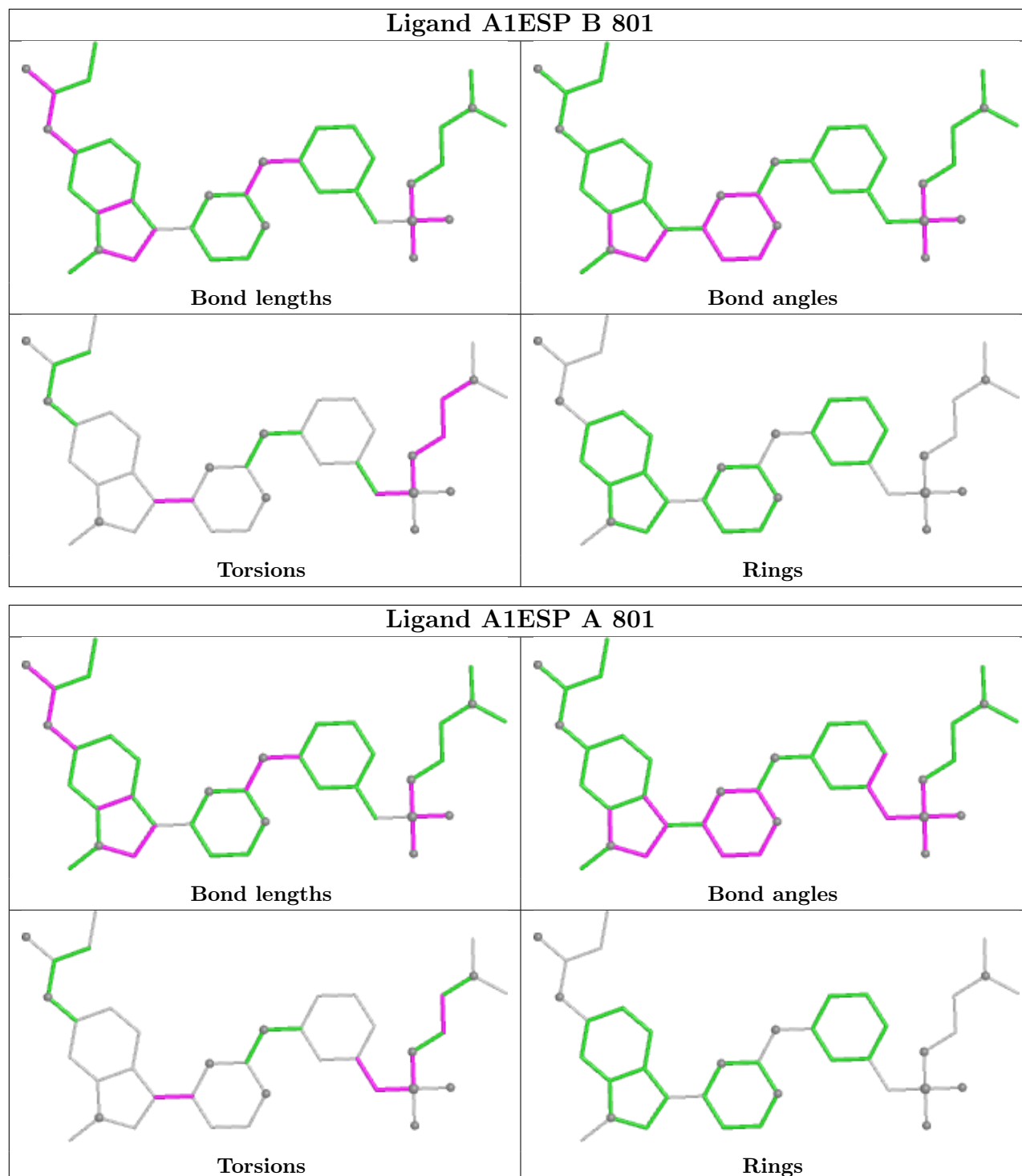
There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	GOL	9	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	278/303 (91%)	0.29	12 (4%) 40 39	24, 39, 68, 87	0
1	B	280/303 (92%)	0.55	27 (9%) 13 12	21, 42, 83, 112	0
All	All	558/606 (92%)	0.42	39 (6%) 22 21	21, 41, 78, 112	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	522	ASP	4.0
1	B	661	THR	3.9
1	B	763	LEU	3.8
1	B	583	GLY	3.8
1	B	586	TYR	3.7
1	A	763	LEU	3.3
1	B	582	PRO	3.3
1	B	665	LEU	3.2
1	A	594	PRO	3.1
1	B	506	ASP	3.0
1	B	508	PRO	2.9
1	B	648	ALA	2.8
1	B	492	PHE	2.8
1	B	649	ARG	2.7
1	A	504	ASP	2.7
1	A	761	LEU	2.7
1	A	466	TYR	2.6
1	B	663	GLY	2.6
1	B	727	ASN	2.6
1	A	679	VAL	2.6
1	B	505	LYS	2.6
1	B	466	TYR	2.5
1	A	491	CYS	2.4
1	B	584	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	676	PHE	2.3
1	B	726	ALA	2.3
1	A	623	ILE	2.3
1	B	511	ALA	2.3
1	B	761	LEU	2.2
1	B	501	VAL	2.2
1	B	509	LYS	2.2
1	B	595	GLU	2.1
1	A	730	ASN	2.1
1	B	594	PRO	2.1
1	B	465	GLU	2.0
1	B	512	VAL	2.0
1	B	502	GLY	2.0
1	A	584	MET	2.0
1	A	762	THR	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](#)

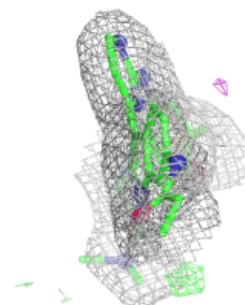
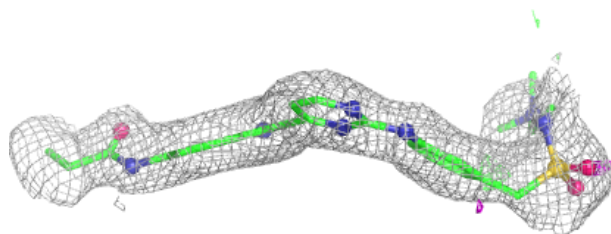
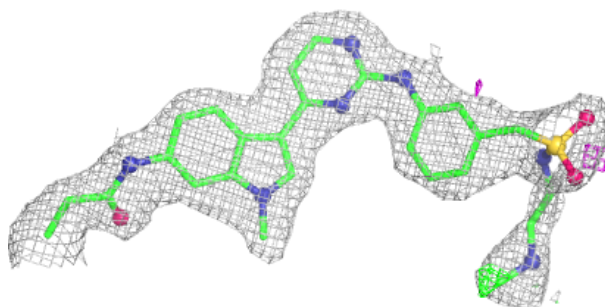
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	B	802	6/6	0.69	0.17	49,56,64,65	0
3	GOL	A	802	6/6	0.71	0.19	43,49,52,56	0
2	A1ESP	B	801	38/38	0.88	0.11	27,42,75,78	0
2	A1ESP	A	801	38/38	0.90	0.11	26,39,66,72	0

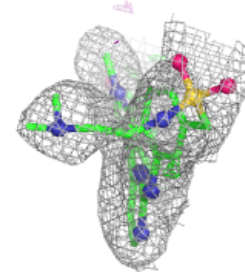
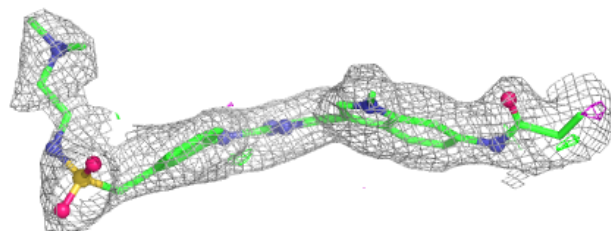
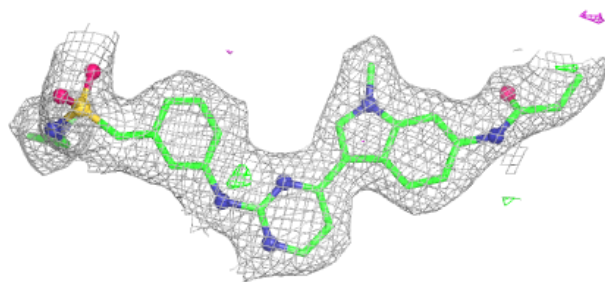
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1ESP 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 A1ESP 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.