



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:23 pm BST

PDB ID : 5VND
Title : Crystal structure of FGFR1-Y563C (FGFR4 surrogate) covalently bound to H3B-6527
Authors : Tsai, J.H.C.; Reynolds, D.; Fekkes, P.; Smith, P.; Larsen, N.A.
Deposited on : 2017-04-30
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

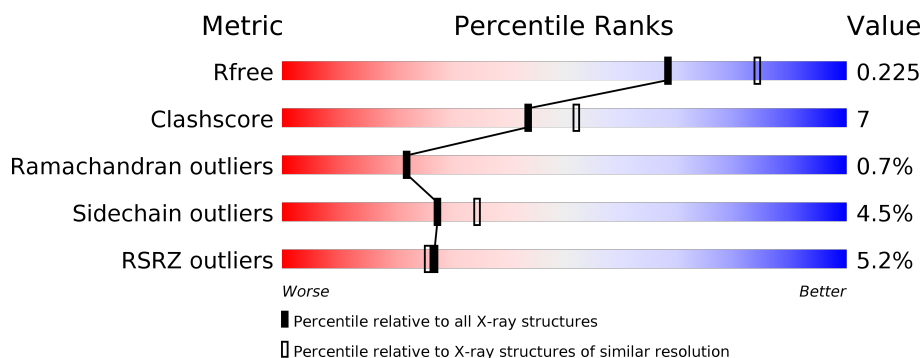
1 Overall quality at a glance ⓘ

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 on 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	309	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>• •</div> </div> </div>
1	B	309	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>• 5%</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
4	EDO	A	811	-	-	X	-
4	EDO	B	806	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5106 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.

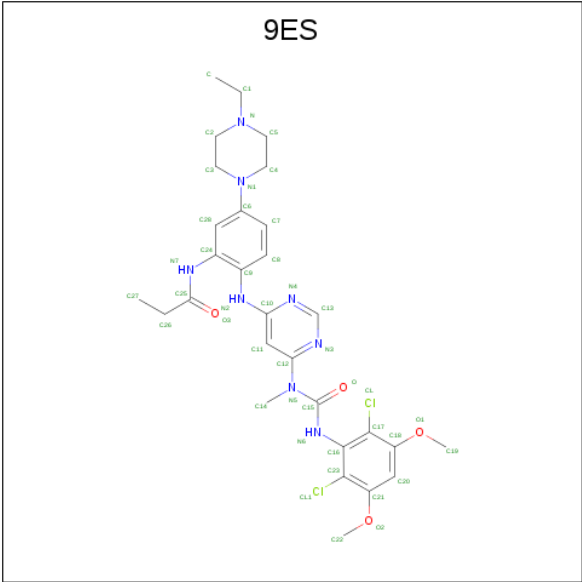
- Molecule 1 is a protein called Fibroblast growth factor receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	1	0
			2381	1512	408	443	18			
1	B	295	Total	C	N	O	S	0	0	0
			2314	1470	394	432	18			

There are 8 discrepancies between the modelled and reference sequences:

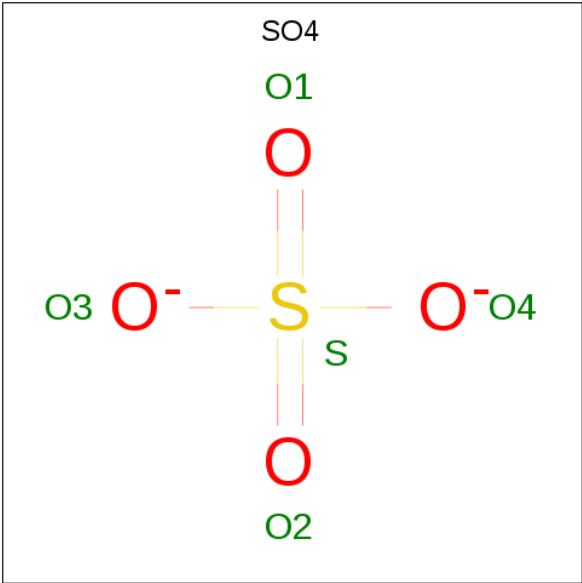
Chain	Residue	Modelled	Actual	Comment	Reference
A	457	GLY	-	expression tag	UNP P11362
A	488	ALA	CYS	engineered mutation	UNP P11362
A	563	CYS	TYR	engineered mutation	UNP P11362
A	584	SER	CYS	engineered mutation	UNP P11362
B	457	GLY	-	expression tag	UNP P11362
B	488	ALA	CYS	engineered mutation	UNP P11362
B	563	CYS	TYR	engineered mutation	UNP P11362
B	584	SER	CYS	engineered mutation	UNP P11362

- Molecule 2 is N-{2-[(6-{[(2,6-dichloro-3,5-dimethoxyphenyl)carbamoyl](methyl)amino}pyrimidin-4-yl)amino]-5-(4-ethylpiperazin-1-yl)phenyl}propanamide (three-letter code: 9ES) (formula: C₂₉H₃₆Cl₂N₈O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 29	Cl 2	N 8	O 4	0	0
2	B	1	Total 43	C 29	Cl 2	N 8	O 4	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



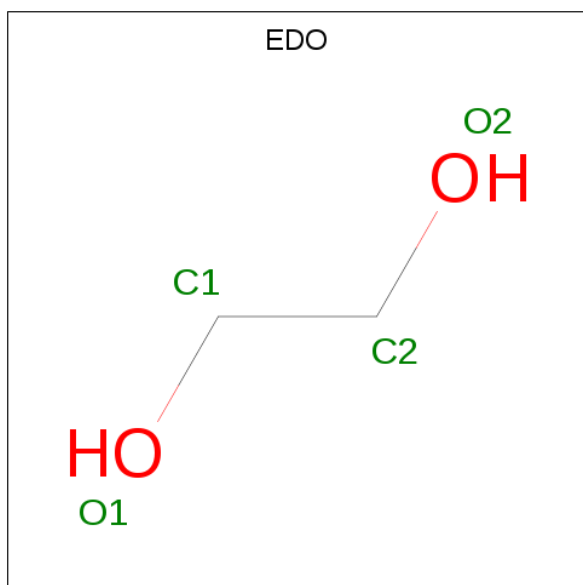
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

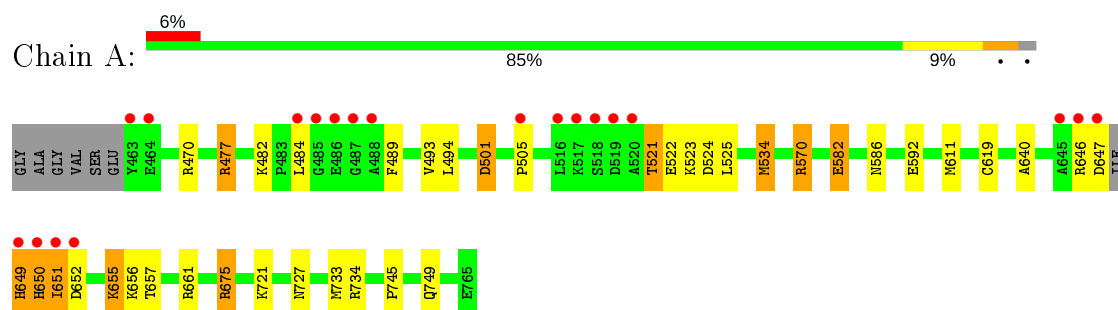
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	124	Total 124	O 124	0	0
5	B	121	Total 121	O 121	0	0

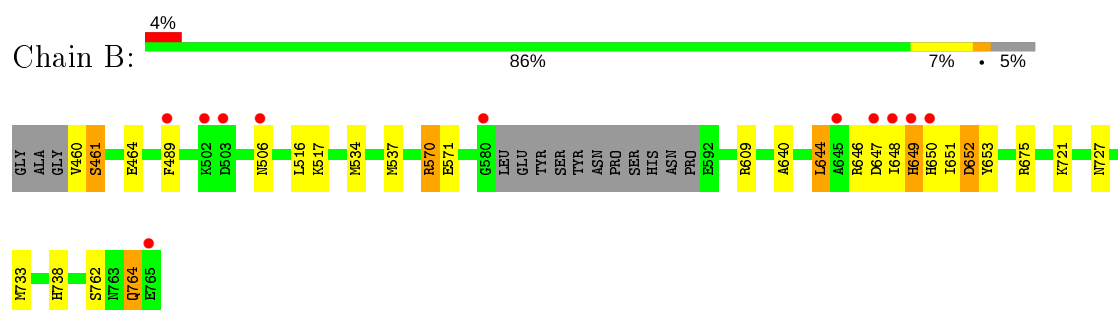
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 1



- Molecule 1: Fibroblast growth factor receptor 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.49Å 58.92Å 65.94Å 90.00° 107.59° 90.00°	Depositor
Resolution (Å)	99.37 – 2.20 46.39 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.9 (99.37-2.20) 99.4 (46.39-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.178 , 0.223 0.187 , 0.225	Depositor DCC
R_{free} test set	2339 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5106	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 9ES, SO4, EDO

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	0.83	0/2436	0.95	5/3298 (0.2%)
1	B	0.87	1/2360 (0.0%)	0.97	4/3193 (0.1%)
All	All	0.85	1/4796 (0.0%)	0.96	9/6491 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	571	GLU	CD-OE1	5.19	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	570	ARG	NE-CZ-NH2	14.88	127.74	120.30
1	B	570	ARG	NE-CZ-NH1	-13.65	113.48	120.30
1	A	570	ARG	NE-CZ-NH2	-12.40	114.10	120.30
1	A	570	ARG	NE-CZ-NH1	12.04	126.32	120.30
1	B	733	MET	CG-SD-CE	-7.45	88.28	100.20
1	B	537	MET	CA-CB-CG	6.69	124.68	113.30
1	A	675	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	733	MET	CG-SD-CE	-5.21	91.87	100.20
1	A	734	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2381	0	2356	37	0
1	B	2314	0	2303	22	0
2	A	43	0	0	3	0
2	B	43	0	0	2	0
3	A	10	0	0	0	0
3	B	10	0	0	1	0
4	A	36	0	54	8	0
4	B	24	0	36	4	0
5	A	124	0	0	5	0
5	B	121	0	0	3	0
All	All	5106	0	4749	64	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 7.

All (64) 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)
4:B:806:EDO:H12	5:B:901:HOH:O	1.29	1.27
4:B:806:EDO:C1	5:B:901:HOH:O	1.81	1.16
1:A:749:GLN:HG2	4:A:811:EDO:C1	2.05	0.86
1:B:649:HIS:N	1:B:650:HIS:HA	2.01	0.74
1:A:619:CYS:SG	5:A:1012:HOH:O	2.45	0.73
1:A:749:GLN:HG2	4:A:811:EDO:H12	1.73	0.71
1:B:644:LEU:N	1:B:644:LEU:HD23	2.05	0.71
1:A:651:ILE:HG23	1:A:652:ASP:H	1.57	0.69
2:A:801:9ES:N3	2:A:801:9ES:N6	2.37	0.69
1:A:749:GLN:HG2	4:A:811:EDO:H11	1.72	0.69
1:B:762:SER:OG	1:B:764:GLN:OE1	2.08	0.68
4:B:806:EDO:C2	5:B:901:HOH:O	2.23	0.68
1:A:655:LYS:HE2	1:A:656:LYS:N	2.10	0.67
2:B:801:9ES:N3	2:B:801:9ES:N6	2.43	0.66
1:A:651:ILE:HG12	1:A:652:ASP:H	1.61	0.64
1:B:651:ILE:HD12	1:B:652:ASP:H	1.62	0.64
1:B:646:ARG:O	1:B:647:ASP:HB2	2.00	0.61
1:A:651:ILE:HG12	1:A:652:ASP:N	2.16	0.61
1:A:651:ILE:HG23	1:A:652:ASP:N	2.15	0.61
1:A:657:THR:HG23	1:A:661:ARG:O	2.01	0.60
1:A:586:ASN:CB	5:A:1001:HOH:O	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:ILE:HG23	1:B:653:TYR:CE1	2.38	0.58
1:A:655:LYS:CE	1:A:656:LYS:H	2.17	0.57
1:A:650:HIS:O	1:A:651:ILE:HG22	2.05	0.57
1:A:745:PRO:HA	4:A:811:EDO:H22	1.86	0.56
1:A:655:LYS:HA	1:A:655:LYS:HE3	1.86	0.56
1:A:655:LYS:HE2	1:A:656:LYS:H	1.69	0.56
1:B:651:ILE:HD12	1:B:652:ASP:N	2.21	0.56
1:B:648:ILE:HG13	1:B:648:ILE:O	2.06	0.55
1:A:611:MET:HE3	5:A:961:HOH:O	2.06	0.55
1:B:651:ILE:CG2	1:B:653:TYR:CE1	2.91	0.54
1:B:461:SER:HA	1:B:464:GLU:O	2.08	0.53
1:A:493:VAL:HG22	1:A:494:LEU:O	2.08	0.53
1:B:644:LEU:H	1:B:644:LEU:HD23	1.73	0.53
1:B:649:HIS:H	1:B:650:HIS:HA	1.74	0.52
2:A:801:9ES:N2	2:A:801:9ES:C26	2.73	0.51
1:A:655:LYS:CE	1:A:656:LYS:N	2.73	0.51
1:B:640:ALA:HB1	2:B:801:9ES:CL1	2.47	0.51
1:A:646:ARG:CB	1:A:647:ASP:HA	2.42	0.50
1:A:749:GLN:CG	4:A:811:EDO:H12	2.41	0.50
1:B:649:HIS:N	1:B:650:HIS:CA	2.73	0.49
1:A:649:HIS:CD2	1:A:649:HIS:N	2.80	0.49
1:B:516:LEU:O	4:B:806:EDO:H11	2.13	0.48
1:A:501:ASP:N	1:A:501:ASP:OD1	2.32	0.48
1:B:649:HIS:H	1:B:650:HIS:CA	2.27	0.48
1:A:640:ALA:HB1	2:A:801:9ES:CL1	2.51	0.48
1:A:749:GLN:CG	4:A:811:EDO:C1	2.87	0.47
1:B:460:VAL:HG13	1:B:461:SER:N	2.31	0.46
1:A:652:ASP:HB3	1:A:655:LYS:HB2	1.97	0.45
1:A:477:ARG:HA	1:A:477:ARG:NE	2.31	0.45
1:A:651:ILE:CG2	1:A:652:ASP:H	2.25	0.43
1:B:649:HIS:CB	1:B:675:ARG:NH2	2.80	0.43
1:B:570:ARG:HD3	3:B:802:SO4:O1	2.18	0.43
1:A:521:THR:OG1	1:A:524:ASP:CB	2.67	0.43
1:A:534:MET:HE3	5:A:1012:HOH:O	2.17	0.43
1:A:505:PRO:HD2	5:A:987:HOH:O	2.18	0.42
1:A:582:GLU:OE2	1:B:738:HIS:CE1	2.73	0.42
1:A:727:ASN:HB2	4:A:808:EDO:H11	2.02	0.42
1:A:521:THR:OG1	1:A:524:ASP:HB2	2.19	0.42
1:B:721:LYS:NZ	1:B:727:ASN:OD1	2.48	0.42
1:B:489:PHE:HA	1:B:517:LYS:HD3	2.03	0.41
1:A:651:ILE:CG1	1:A:652:ASP:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:GLN:CG	4:A:811:EDO:H11	2.47	0.41
1:A:484:LEU:HD11	1:A:494:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	299/309 (97%)	289 (97%)	9 (3%)	1 (0%)	41	46
1	B	291/309 (94%)	283 (97%)	5 (2%)	3 (1%)	15	14
All	All	590/618 (96%)	572 (97%)	14 (2%)	4 (1%)	22	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	649	HIS
1	B	461	SER
1	B	652	ASP
1	A	651	ILE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/269 (96%)	240 (93%)	18 (7%)	15	16
1	B	250/269 (93%)	245 (98%)	5 (2%)	55	69
All	All	508/538 (94%)	485 (96%)	23 (4%)	27	34

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	470	ARG
1	A	477	ARG
1	A	482	LYS
1	A	489	PHE
1	A	501	ASP
1	A	521	THR
1	A	522	GLU
1	A	523	LYS
1	A	525	LEU
1	A	534	MET
1	A	570	ARG
1	A	582	GLU
1	A	592	GLU
1	A	649	HIS
1	A	650	HIS
1	A	655	LYS
1	A	675	ARG
1	A	721	LYS
1	B	506	ASN
1	B	534	MET
1	B	609	ARG
1	B	644	LEU
1	B	764	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	649	HIS
1	A	749	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

21 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	$\# Z > 2$
2	9ES	A	801	1	45,46,46	1.52	5 (11%)	57,64,64	2.53	23 (40%)
3	SO4	B	803	-	4,4,4	0.47	0	6,6,6	0.29	0
4	EDO	A	804	-	3,3,3	0.45	0	2,2,2	0.39	0
4	EDO	A	807	-	3,3,3	0.44	0	2,2,2	0.90	0
4	EDO	B	807	-	3,3,3	0.58	0	2,2,2	0.49	0
4	EDO	A	806	-	3,3,3	0.54	0	2,2,2	0.58	0
4	EDO	A	810	-	3,3,3	0.67	0	2,2,2	0.53	0
4	EDO	A	811	-	3,3,3	0.27	0	2,2,2	1.36	0
4	EDO	B	804	-	3,3,3	0.21	0	2,2,2	0.82	0
4	EDO	A	809	-	3,3,3	0.44	0	2,2,2	0.49	0
4	EDO	B	805	-	3,3,3	0.74	0	2,2,2	0.53	0
2	9ES	B	801	1	45,46,46	1.44	6 (13%)	57,64,64	2.66	15 (26%)
4	EDO	A	805	-	3,3,3	0.39	0	2,2,2	1.02	0
3	SO4	A	802	-	4,4,4	0.30	0	6,6,6	0.37	0
3	SO4	A	803	-	4,4,4	0.90	0	6,6,6	0.89	0
4	EDO	A	812	-	3,3,3	0.69	0	2,2,2	0.63	0
3	SO4	B	802	-	4,4,4	0.28	0	6,6,6	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	808	-	3,3,3	0.75	0	2,2,2	0.41	0
4	EDO	A	808	-	3,3,3	0.62	0	2,2,2	0.12	0
4	EDO	B	806	-	3,3,3	0.57	0	2,2,2	0.36	0
4	EDO	B	809	-	3,3,3	0.49	0	2,2,2	0.52	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	9ES	A	801	1	-	7/32/42/42	0/4/4/4
4	EDO	A	804	-	-	1/1/1/1	-
4	EDO	A	807	-	-	1/1/1/1	-
4	EDO	B	807	-	-	1/1/1/1	-
4	EDO	A	806	-	-	1/1/1/1	-
4	EDO	A	810	-	-	1/1/1/1	-
4	EDO	A	811	-	-	0/1/1/1	-
4	EDO	B	804	-	-	0/1/1/1	-
4	EDO	A	809	-	-	0/1/1/1	-
4	EDO	B	805	-	-	0/1/1/1	-
2	9ES	B	801	1	-	4/32/42/42	0/4/4/4
4	EDO	A	805	-	-	1/1/1/1	-
4	EDO	A	812	-	-	1/1/1/1	-
4	EDO	B	808	-	-	1/1/1/1	-
4	EDO	A	808	-	-	1/1/1/1	-
4	EDO	B	806	-	-	1/1/1/1	-
4	EDO	B	809	-	-	0/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	9ES	C24-C9	5.37	1.50	1.40
2	B	801	9ES	C24-C9	4.32	1.48	1.40
2	B	801	9ES	C16-N6	-4.31	1.35	1.43
2	A	801	9ES	C18-C17	3.73	1.46	1.40
2	B	801	9ES	C10-N2	-3.08	1.33	1.38
2	A	801	9ES	C16-N6	-2.86	1.37	1.43
2	B	801	9ES	C24-N7	-2.85	1.36	1.41
2	A	801	9ES	C16-C17	2.57	1.46	1.40
2	A	801	9ES	C24-N7	-2.41	1.37	1.41
2	B	801	9ES	C21-C23	2.21	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	9ES	C15-N5	2.06	1.40	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	9ES	C13-N3-C12	12.88	126.19	114.94
2	A	801	9ES	C13-N3-C12	10.09	123.76	114.94
2	B	801	9ES	N3-C13-N4	-5.40	120.16	128.60
2	B	801	9ES	N3-C12-N5	5.16	119.51	115.28
2	A	801	9ES	C9-C24-N7	5.10	129.24	119.56
2	B	801	9ES	C11-C12-N3	-4.69	114.62	122.73
2	B	801	9ES	C22-O2-C21	4.64	124.54	117.53
2	A	801	9ES	C11-C12-N5	4.22	126.97	122.48
2	A	801	9ES	N3-C13-N4	-4.09	122.21	128.60
2	A	801	9ES	C4-N1-C3	4.04	120.44	111.52
2	A	801	9ES	C26-C25-N7	3.95	125.31	114.75
2	B	801	9ES	C9-C24-N7	-3.87	112.23	119.56
2	A	801	9ES	C11-C12-N3	-3.83	116.10	122.73
2	A	801	9ES	C28-C24-C9	-3.59	116.05	119.50
2	A	801	9ES	C24-C9-N2	3.54	125.69	118.83
2	B	801	9ES	C14-N5-C15	3.49	125.58	118.22
2	A	801	9ES	C16-N6-C15	3.30	127.27	122.26
2	B	801	9ES	C17-C16-C23	-3.22	112.08	118.44
2	B	801	9ES	C4-N1-C3	3.16	118.48	111.52
2	B	801	9ES	C11-C12-N5	3.14	125.82	122.48
2	A	801	9ES	C19-O1-C18	3.06	122.15	117.53
2	A	801	9ES	C8-C9-N2	-3.05	115.10	121.39
2	B	801	9ES	C19-O1-C18	3.03	122.11	117.53
2	B	801	9ES	C28-C24-N7	3.01	129.87	121.90
2	A	801	9ES	C17-C16-C23	-2.96	112.60	118.44
2	A	801	9ES	C14-N5-C15	2.82	124.18	118.22
2	B	801	9ES	C16-N6-C15	2.76	126.46	122.26
2	A	801	9ES	C28-C24-N7	-2.72	114.71	121.90
2	A	801	9ES	C11-C10-N2	2.69	128.76	120.24
2	B	801	9ES	C5-C4-N1	-2.68	105.49	110.70
2	A	801	9ES	O3-C25-C26	-2.55	114.97	122.08
2	B	801	9ES	C20-C21-C23	-2.47	117.67	120.76
2	A	801	9ES	N2-C10-N4	-2.33	109.68	116.81
2	A	801	9ES	C7-C8-C9	2.22	123.94	119.64
2	A	801	9ES	O3-C25-N7	-2.22	119.58	123.63
2	A	801	9ES	C3-C2-N	-2.19	106.15	110.64
2	A	801	9ES	C7-C6-N1	-2.19	118.36	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	9ES	C24-N7-C25	2.14	134.09	126.57

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	9ES	O3-C25-N7-C24
2	A	801	9ES	C26-C25-N7-C24
2	A	801	9ES	C28-C24-N7-C25
2	A	801	9ES	C9-C24-N7-C25
4	A	807	EDO	O1-C1-C2-O2
4	B	808	EDO	O1-C1-C2-O2
2	A	801	9ES	C-C1-N-C2
2	A	801	9ES	C-C1-N-C5
2	B	801	9ES	C-C1-N-C2
2	B	801	9ES	N7-C25-C26-C27
4	A	812	EDO	O1-C1-C2-O2
4	B	806	EDO	O1-C1-C2-O2
2	B	801	9ES	O3-C25-C26-C27
4	A	806	EDO	O1-C1-C2-O2
4	A	805	EDO	O1-C1-C2-O2
2	B	801	9ES	C24-C9-N2-C10
4	B	807	EDO	O1-C1-C2-O2
4	A	810	EDO	O1-C1-C2-O2
2	A	801	9ES	C24-C9-N2-C10
4	A	804	EDO	O1-C1-C2-O2
4	A	808	EDO	O1-C1-C2-O2

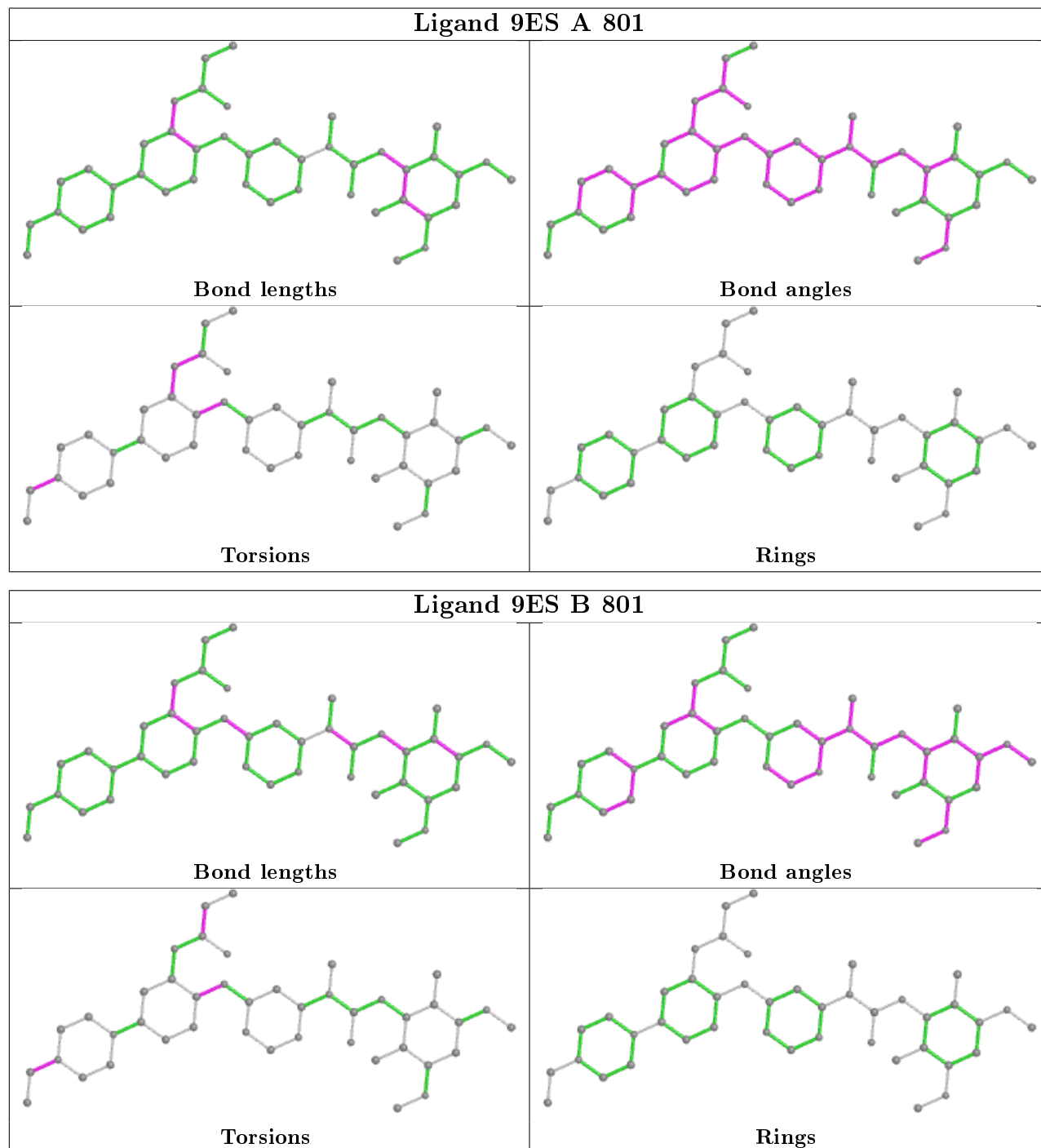
There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	9ES	3	0
4	A	811	EDO	7	0
2	B	801	9ES	2	0
3	B	802	SO4	1	0
4	A	808	EDO	1	0
4	B	806	EDO	4	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	302/309 (97%)	0.07	20 (6%) 18 17	28, 47, 105, 143	0
1	B	295/309 (95%)	-0.25	11 (3%) 41 39	29, 44, 94, 141	0
All	All	597/618 (96%)	-0.09	31 (5%) 27 26	28, 45, 103, 143	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	503	ASP	6.1
1	A	650	HIS	6.1
1	A	485	GLY	5.0
1	A	520	ALA	4.9
1	A	651	ILE	4.9
1	A	645	ALA	4.8
1	B	489	PHE	4.4
1	A	647	ASP	4.3
1	A	649	HIS	4.3
1	A	488	ALA	3.8
1	A	464	GLU	3.5
1	A	486	GLU	3.4
1	B	647	ASP	3.2
1	A	487	GLY	3.2
1	B	580	GLY	3.0
1	A	518	SER	2.9
1	A	517	LYS	2.9
1	A	463	TYR	2.8
1	B	649	HIS	2.8
1	A	505	PRO	2.7
1	B	645	ALA	2.7
1	A	652	ASP	2.7
1	B	506	ASN	2.7
1	A	519	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	516	LEU	2.6
1	B	648	ILE	2.5
1	B	650	HIS	2.4
1	A	646	ARG	2.3
1	B	502	LYS	2.3
1	A	484	LEU	2.2
1	B	765	GLU	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 carbohydrates 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
4	EDO	A	812	4/4	0.72	0.24	54,71,71,72	0
4	EDO	A	810	4/4	0.74	0.17	68,71,72,72	0
4	EDO	B	808	4/4	0.75	0.18	57,71,71,72	0
4	EDO	A	808	4/4	0.78	0.17	54,56,67,68	0
4	EDO	B	805	4/4	0.81	0.15	56,67,68,70	0
4	EDO	A	807	4/4	0.83	0.21	65,67,73,76	0
4	EDO	B	809	4/4	0.88	0.27	72,74,74,81	0
4	EDO	A	811	4/4	0.89	0.30	50,57,61,65	0
4	EDO	A	809	4/4	0.90	0.10	69,71,76,77	0
4	EDO	B	807	4/4	0.91	0.15	66,68,70,71	0
4	EDO	A	806	4/4	0.93	0.15	55,58,60,60	0
4	EDO	B	806	4/4	0.94	0.24	58,71,76,85	0
2	9ES	A	801	43/43	0.95	0.13	38,50,108,112	0
2	9ES	B	801	43/43	0.96	0.12	34,45,98,101	0
3	SO4	A	803	5/5	0.96	0.11	56,66,73,81	0
3	SO4	B	803	5/5	0.96	0.29	74,75,99,109	0

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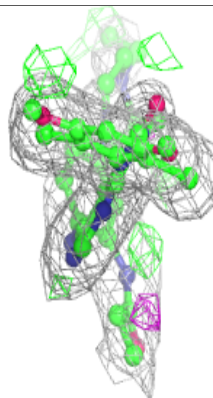
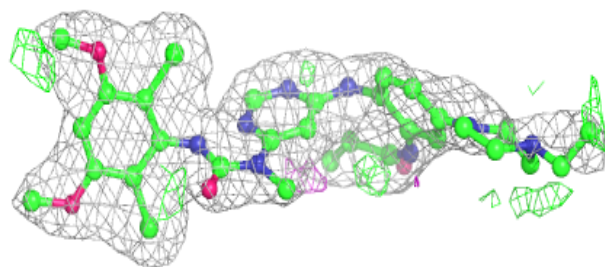
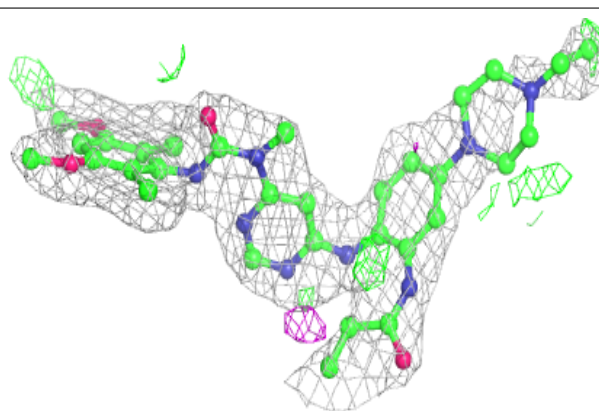
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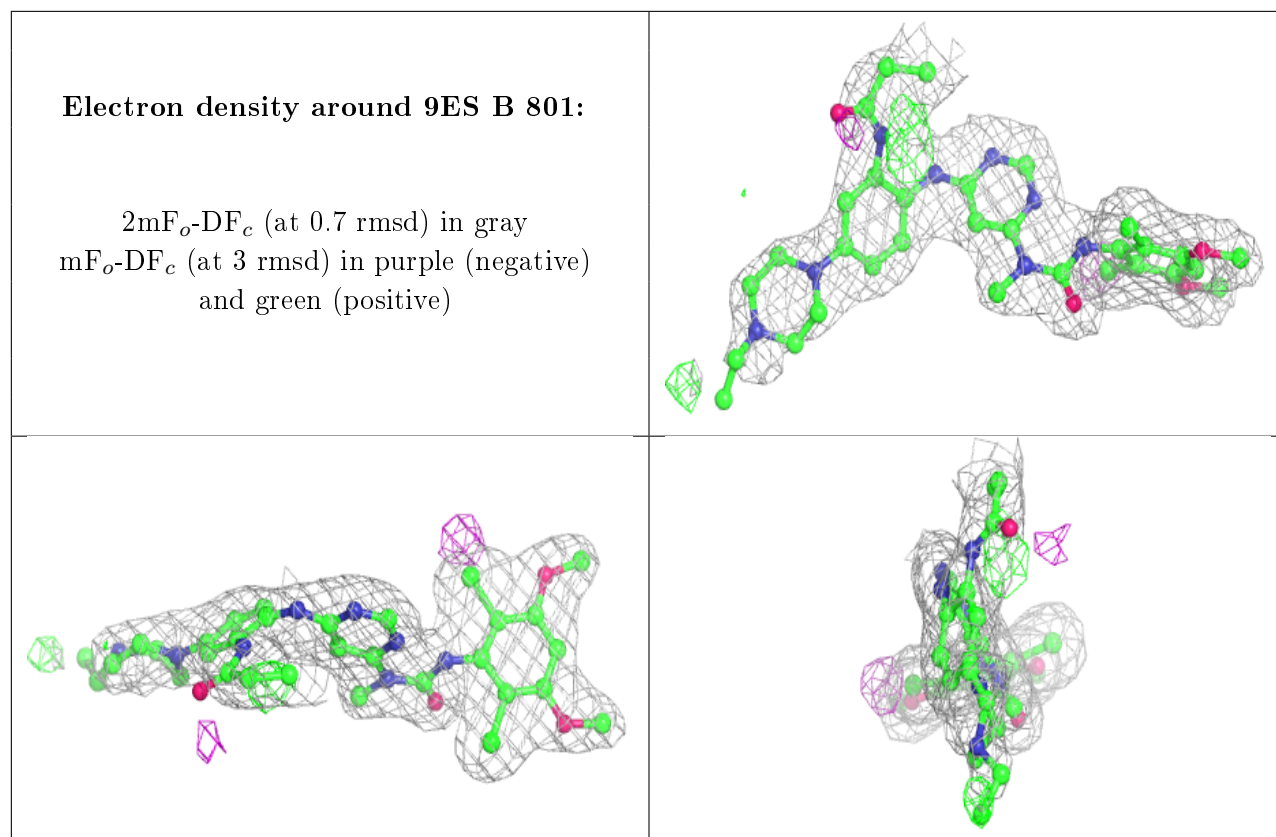
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	802	5/5	0.97	0.07	59,67,71,71	0
4	EDO	B	804	4/4	0.97	0.15	40,40,40,51	0
4	EDO	A	804	4/4	0.97	0.16	37,40,42,50	0
4	EDO	A	805	4/4	0.98	0.12	37,38,40,43	0
3	SO4	B	802	5/5	0.99	0.11	47,58,65,67	0

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 9ES 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.