



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 08:24 am BST

PDB ID : 3QGD  
Title : Crystal structure of the hepatitis C virus NS5B RNA-dependent RNA polymerase complex with (2E)-3-(4-{{(1-{{(13-cyclohexyl-6-oxo-6,7-dihydro-5H-indolo[1,2-d][1,4]benzodiazepin-10-yl)carbonyl}amino}cyclopentyl)carbonyl}amino}phenyl)prop-2-enoic acid and (2R)-4-(2,6-dimethoxypyrimidin-4-yl)-1-[(4-ethylphenyl)sulfonyl]-N-(4-methoxybenzyl)piperazine-2-carboxamide  
Authors : Sheriff, S.  
Deposited on : 2011-01-24  
Resolution : 2.60 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](mailto: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.

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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

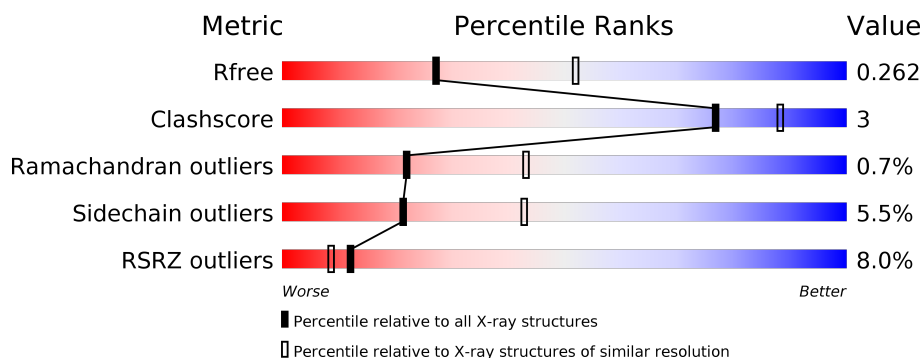
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	574	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>6%</div> </div> </div>
1	B	574	<div> <div>9%</div> <div> <div></div> <div>80%</div> <div>8%</div> <div>10%</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8421 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.

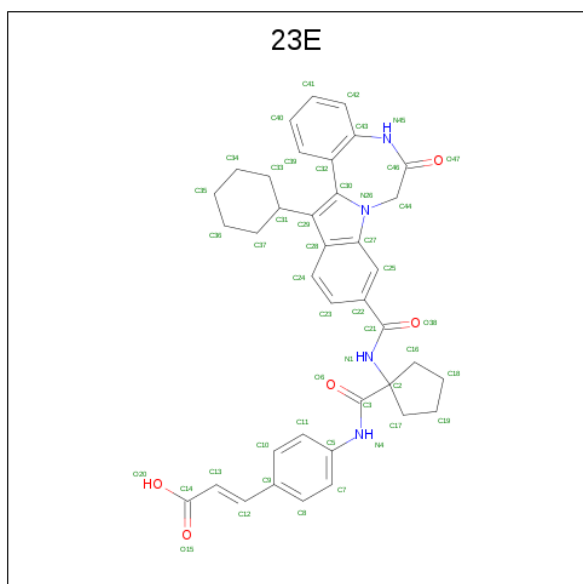
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4162	2625	736	769	32			
1	B	515	Total	C	N	O	S	0	0	0
			3999	2518	712	737	32			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING METHIONINE	UNP Q9WMX2
B	0	MET	-	INITIATING METHIONINE	UNP Q9WMX2

- Molecule 2 is (2E)-3-(4-{{(1-{{(13-cyclohexyl-6-oxo-6,7-dihydro-5H-indolo[1,2-d][1,4]benzodiazepin-10-yl)carbonyl}amino}cyclopentyl)carbonyl}amino}phenyl)prop-2-enoic acid (three-letter code: 23E) (formula: C<sub>38</sub>H<sub>38</sub>N<sub>4</sub>O<sub>5</sub>).



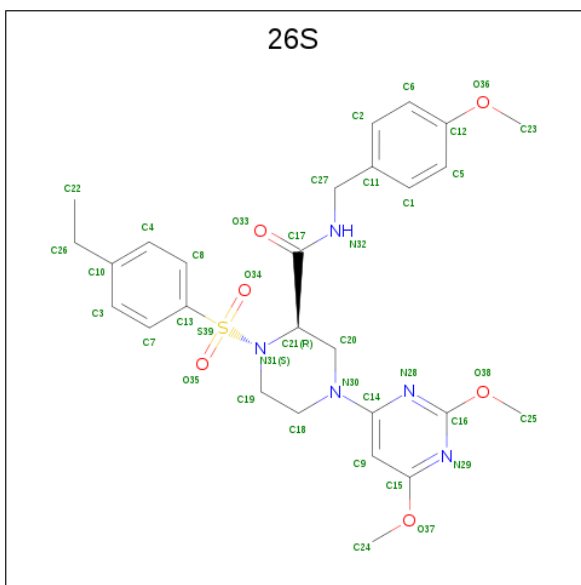
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			47	38	4	5		
2	B	1	Total	C	N	O	0	0
			47	38	4	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
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 (2R)-4-(2,6-dimethoxypyrimidin-4-yl)-1-[(4-ethylphenyl)sulfonyl]-N-(4-methoxybenzyl)piperazine-2-carboxamide (three-letter code: 26S) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>5</sub>O<sub>6</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			39	27	5	6	1		

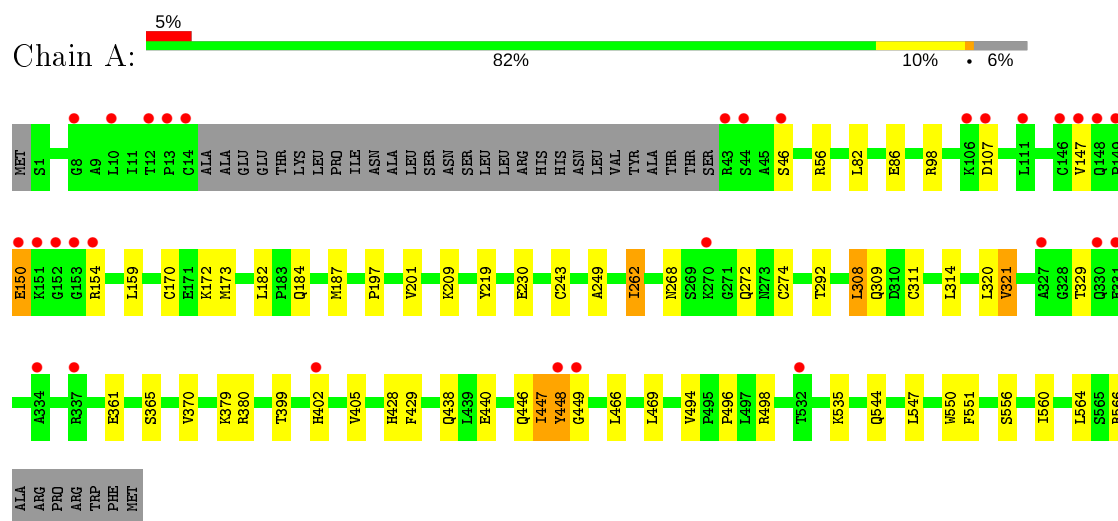
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	61	Total O 61 61	0	0
5	B	36	Total O 36 36	0	0

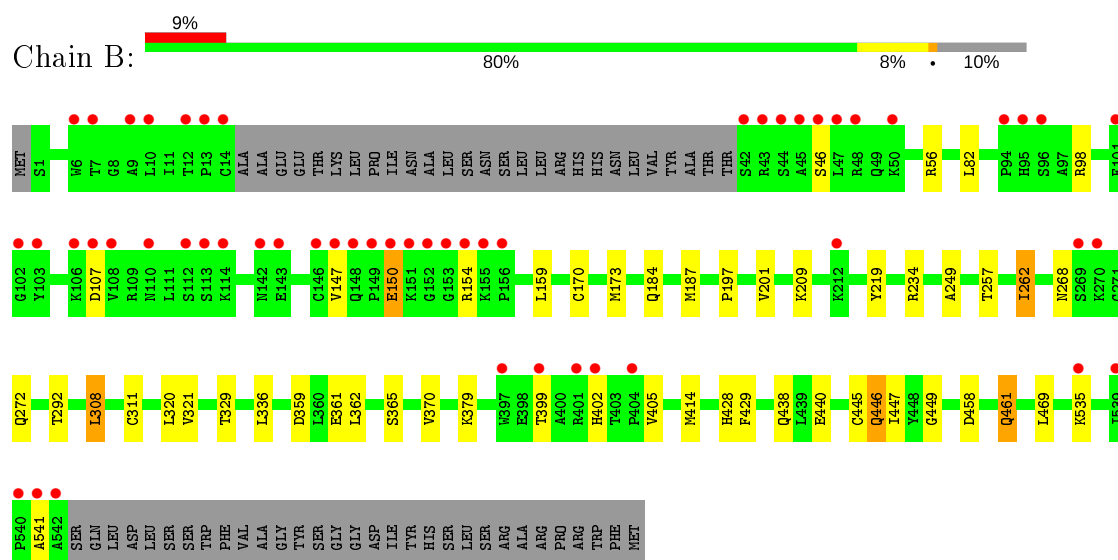
### 3 Residue-property plots [i](#)

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: RNA-directed RNA polymerase



#### • Molecule 1: RNA-directed RNA polymerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.00Å 91.60Å 231.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.56 – 2.60 43.56 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.3 (43.56-2.60) 97.3 (43.56-2.60)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.61Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.9.7, BUSTER 2.9.7	Depositor
R, $R_{free}$	0.233 , 0.262 0.233 , 0.262	Depositor DCC
$R_{free}$ test set	639 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.1	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8421	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 26S, 23E, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.45	0/4252	0.69	1/5769 (0.0%)
1	B	0.46	0/4083	0.67	0/5537
All	All	0.45	0/8335	0.68	1/11306 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	ILE	C-N-CA	6.91	138.98	121.70

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	4162	0	4156	24	0
1	B	3999	0	4019	25	0
2	A	47	0	37	3	0
2	B	47	0	37	0	0
3	A	10	0	0	0	0
3	B	20	0	0	0	0
4	B	39	0	33	1	0
5	A	61	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	36	0	0	0	0
All	All	8421	0	8282	50	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 3.

All (50) 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:321:VAL:HG21	1:B:365:SER:HB3	1.56	0.85
1:B:321:VAL:HG21	1:B:365:SER:CB	2.14	0.77
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.74	0.68
1:B:321:VAL:CG2	1:B:365:SER:HB3	2.23	0.67
1:A:170:CYS:HA	1:A:173:MET:HE3	1.76	0.66
1:A:405:VAL:HG11	1:A:446:GLN:HG2	1.77	0.66
1:A:308:LEU:HB3	1:A:311:CYS:SG	2.38	0.64
1:B:197:PRO:O	1:B:201:VAL:HG23	1.99	0.63
1:B:308:LEU:HB3	1:B:311:CYS:SG	2.38	0.63
1:B:170:CYS:HA	1:B:173:MET:HE3	1.81	0.62
1:A:197:PRO:O	1:A:201:VAL:HG23	1.99	0.61
1:A:399:THR:HG21	1:A:428:HIS:NE2	2.15	0.61
1:B:399:THR:HG21	1:B:428:HIS:NE2	2.17	0.59
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.86	0.57
1:A:361:GLU:HG2	1:A:370:VAL:O	2.03	0.57
1:A:314:LEU:HB3	1:A:321:VAL:HG23	1.87	0.56
1:B:458:ASP:O	1:B:461:GLN:HG2	2.06	0.56
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.86	0.56
1:B:321:VAL:CG2	1:B:365:SER:CB	2.82	0.54
1:B:361:GLU:HG2	1:B:370:VAL:O	2.09	0.52
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.49	0.51
2:A:601:23E:O6	2:A:601:23E:H7	2.12	0.50
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.94	0.49
1:B:234:ARG:CG	1:B:262:ILE:HD11	2.44	0.48
1:B:257:THR:HG22	1:B:262:ILE:HD12	1.96	0.48
1:A:230:GLU:HG2	1:A:262:ILE:HG23	1.96	0.48
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.96	0.48
1:A:321:VAL:HG11	1:A:365:SER:HB3	1.96	0.47
1:B:414:MET:HG2	1:B:447:ILE:HD12	1.97	0.47
1:A:446:GLN:O	1:A:447:ILE:HD13	2.15	0.46
1:B:268:ASN:ND2	1:B:272:GLN:HG2	2.32	0.45
1:B:359:ASP:HB3	1:B:362:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:PRO:HD2	2:A:601:23E:H13	1.98	0.45
1:A:268:ASN:ND2	1:A:272:GLN:HG2	2.31	0.45
1:B:197:PRO:HA	4:B:602:26S:H6	1.99	0.45
1:B:446:GLN:HB3	1:B:446:GLN:HE21	1.64	0.44
1:A:150:GLU:HG3	1:A:150:GLU:H	1.67	0.44
1:A:321:VAL:CG1	1:A:365:SER:HB3	2.47	0.44
1:B:399:THR:HG23	1:B:429:PHE:CZ	2.54	0.43
1:A:182:LEU:HD12	1:A:243:CYS:SG	2.58	0.43
1:A:187:MET:CE	1:A:292:THR:HG22	2.49	0.43
1:A:399:THR:HG23	1:A:429:PHE:CZ	2.54	0.43
1:A:544:GLN:HG3	1:A:566:ARG:C	2.39	0.43
1:B:234:ARG:HG3	1:B:262:ILE:HD11	2.01	0.42
1:B:405:VAL:HG13	1:B:445:CYS:HA	2.02	0.42
1:B:150:GLU:HG3	1:B:150:GLU:H	1.67	0.41
1:B:170:CYS:HA	1:B:173:MET:CE	2.48	0.41
1:B:187:MET:CE	1:B:292:THR:HG22	2.50	0.41
1:A:466:LEU:HD22	1:A:551:PHE:HE2	1.85	0.41
1:A:494:VAL:HG22	2:A:601:23E:C30	2.51	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	534/574 (93%)	523 (98%)	7 (1%)	4 (1%)	22	43
1	B	511/574 (89%)	500 (98%)	8 (2%)	3 (1%)	25	47
All	All	1045/1148 (91%)	1023 (98%)	15 (1%)	7 (1%)	22	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	449	GLY
1	B	541	ALA
1	A	550	TRP
1	A	147	VAL
1	A	448	TYR
1	B	147	VAL
1	B	449	GLY

### 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	447/486 (92%)	420 (94%)	27 (6%)	19	39
1	B	432/486 (89%)	411 (95%)	21 (5%)	25	48
All	All	879/972 (90%)	831 (94%)	48 (6%)	21	43

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	SER
1	A	56	ARG
1	A	86	GLU
1	A	98	ARG
1	A	107	ASP
1	A	150	GLU
1	A	154	ARG
1	A	159	LEU
1	A	184	GLN
1	A	209	LYS
1	A	262	ILE
1	A	308	LEU
1	A	309	GLN
1	A	321	VAL
1	A	329	THR
1	A	379	LYS
1	A	380	ARG

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Mol	Chain	Res	Type
1	A	402	HIS
1	A	438	GLN
1	A	440	GLU
1	A	448	TYR
1	A	469	LEU
1	A	498	ARG
1	A	535	LYS
1	A	547	LEU
1	A	556	SER
1	A	564	LEU
1	B	46	SER
1	B	56	ARG
1	B	98	ARG
1	B	107	ASP
1	B	150	GLU
1	B	154	ARG
1	B	159	LEU
1	B	184	GLN
1	B	209	LYS
1	B	262	ILE
1	B	308	LEU
1	B	329	THR
1	B	336	LEU
1	B	379	LYS
1	B	402	HIS
1	B	438	GLN
1	B	440	GLU
1	B	446	GLN
1	B	461	GLN
1	B	469	LEU
1	B	535	LYS

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

Mol	Chain	Res	Type
1	B	446	GLN
1	B	461	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 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	B	653	-	4,4,4	0.36	0	6,6,6	0.11	0
3	SO4	B	657	-	4,4,4	0.41	0	6,6,6	0.22	0
3	SO4	A	652	-	4,4,4	0.23	0	6,6,6	0.28	0
3	SO4	B	656	-	4,4,4	0.39	0	6,6,6	0.26	0
4	26S	B	602	-	42,42,42	1.52	5 (11%)	57,59,59	1.08	3 (5%)
3	SO4	B	658	-	4,4,4	0.28	0	6,6,6	0.17	0
3	SO4	A	653	-	4,4,4	0.73	0	6,6,6	0.23	0
2	23E	A	601	-	44,53,53	1.80	4 (9%)	57,77,77	1.40	7 (12%)
2	23E	B	601	-	44,53,53	1.84	5 (11%)	57,77,77	1.61	10 (17%)

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	23E	A	601	-	-	2/22/57/57	0/6/7/7
4	26S	B	602	-	-	0/33/46/46	0/4/4/4
2	23E	B	601	-	-	1/22/57/57	0/6/7/7

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	23E	C29-C28	9.60	1.50	1.40
2	A	601	23E	C29-C28	9.24	1.50	1.40
4	B	602	26S	S39-N31	6.50	1.73	1.63
2	A	601	23E	C25-C22	2.63	1.42	1.37
2	B	601	23E	C44-N26	-2.53	1.46	1.48
2	B	601	23E	C8-C7	2.50	1.43	1.38
2	A	601	23E	C24-C23	2.41	1.41	1.36
4	B	602	26S	O35-S39	2.30	1.46	1.43
2	A	601	23E	C30-C29	-2.20	1.35	1.41
2	B	601	23E	C30-C29	-2.19	1.35	1.41
4	B	602	26S	C17-N32	2.19	1.38	1.33
4	B	602	26S	C15-N29	2.09	1.36	1.33
4	B	602	26S	O34-S39	2.07	1.45	1.43
2	B	601	23E	C9-C12	2.01	1.53	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	23E	C14-C13-C12	4.88	134.13	123.69
2	A	601	23E	C17-C2-C16	-4.65	97.83	103.41
2	B	601	23E	C9-C12-C13	4.31	142.87	125.87
2	A	601	23E	C16-C2-C3	4.09	120.45	110.67
2	B	601	23E	C17-C2-C16	-3.70	98.98	103.41
2	B	601	23E	C23-C24-C28	-3.42	116.38	121.13
2	A	601	23E	C23-C24-C28	-3.25	116.61	121.13
4	B	602	26S	C20-C21-N31	3.22	113.37	108.73
4	B	602	26S	C11-C27-N32	-2.83	106.99	113.05
4	B	602	26S	C18-C19-N31	2.50	111.05	108.96
2	A	601	23E	C3-C2-N1	-2.49	107.27	110.79
2	B	601	23E	C16-C2-C3	2.47	116.57	110.67
2	B	601	23E	C7-C5-N4	2.34	128.26	120.40
2	A	601	23E	C36-C37-C31	-2.25	107.06	111.47
2	B	601	23E	C39-C32-C43	2.24	120.17	117.92
2	A	601	23E	C14-C13-C12	-2.18	119.03	123.69
2	B	601	23E	C5-N4-C3	2.12	130.64	126.78
2	A	601	23E	C22-C25-C27	-2.12	117.19	121.14
2	B	601	23E	C11-C5-N4	-2.04	113.55	120.40
2	B	601	23E	O47-C46-C44	-2.03	117.54	121.72

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	23E	C13-C12-C9-C8
2	A	601	23E	C13-C12-C9-C10
2	B	601	23E	C9-C12-C13-C14

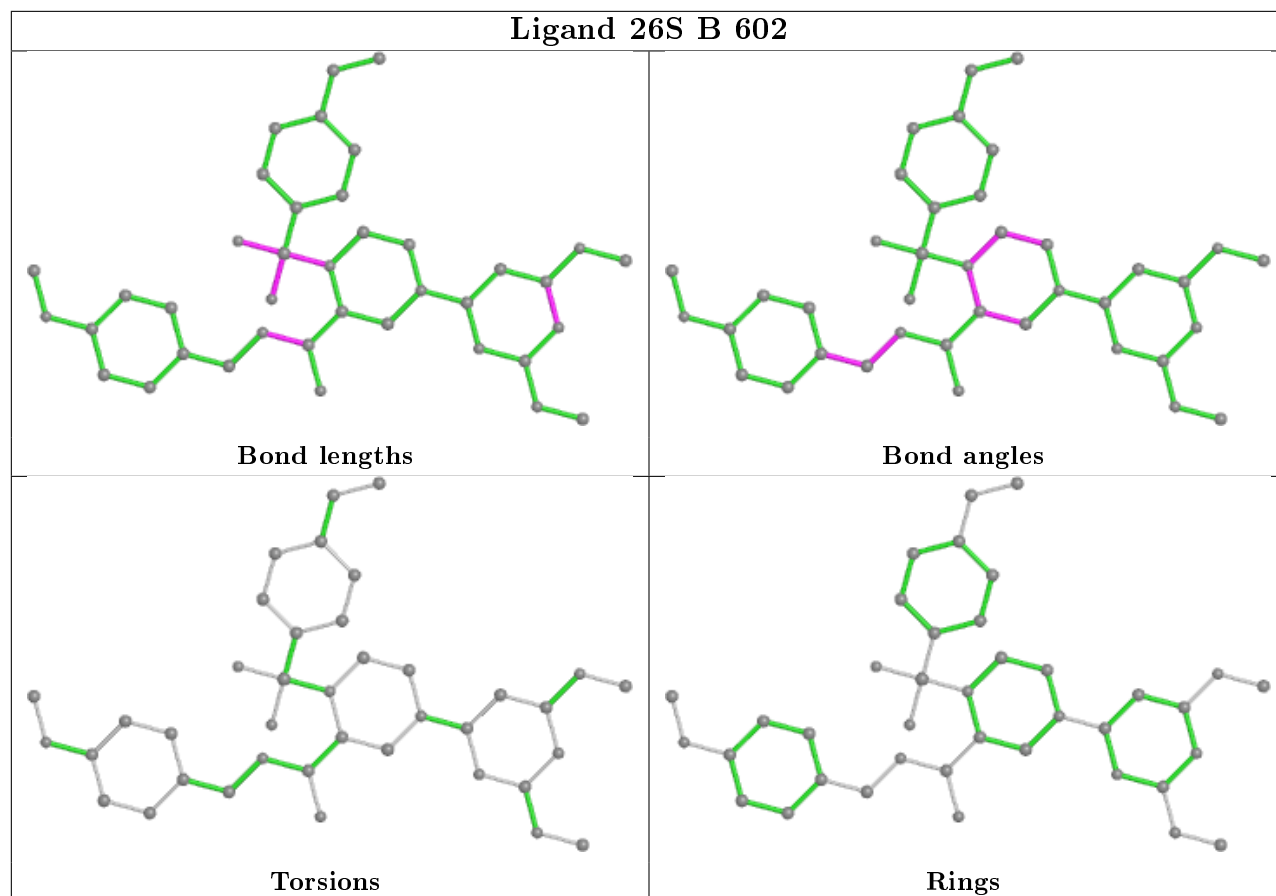
There are no ring outliers.

2 monomers are involved in 4 short contacts:

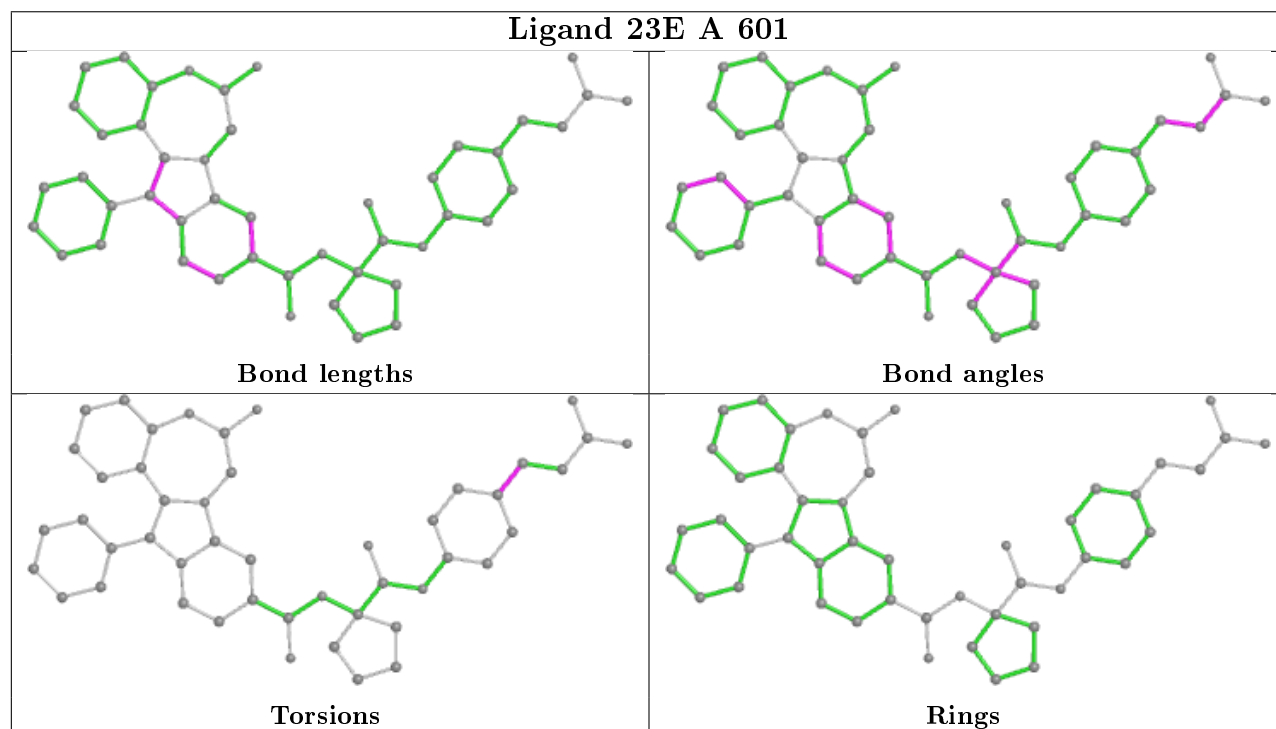
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	26S	1	0
2	A	601	23E	3	0

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.

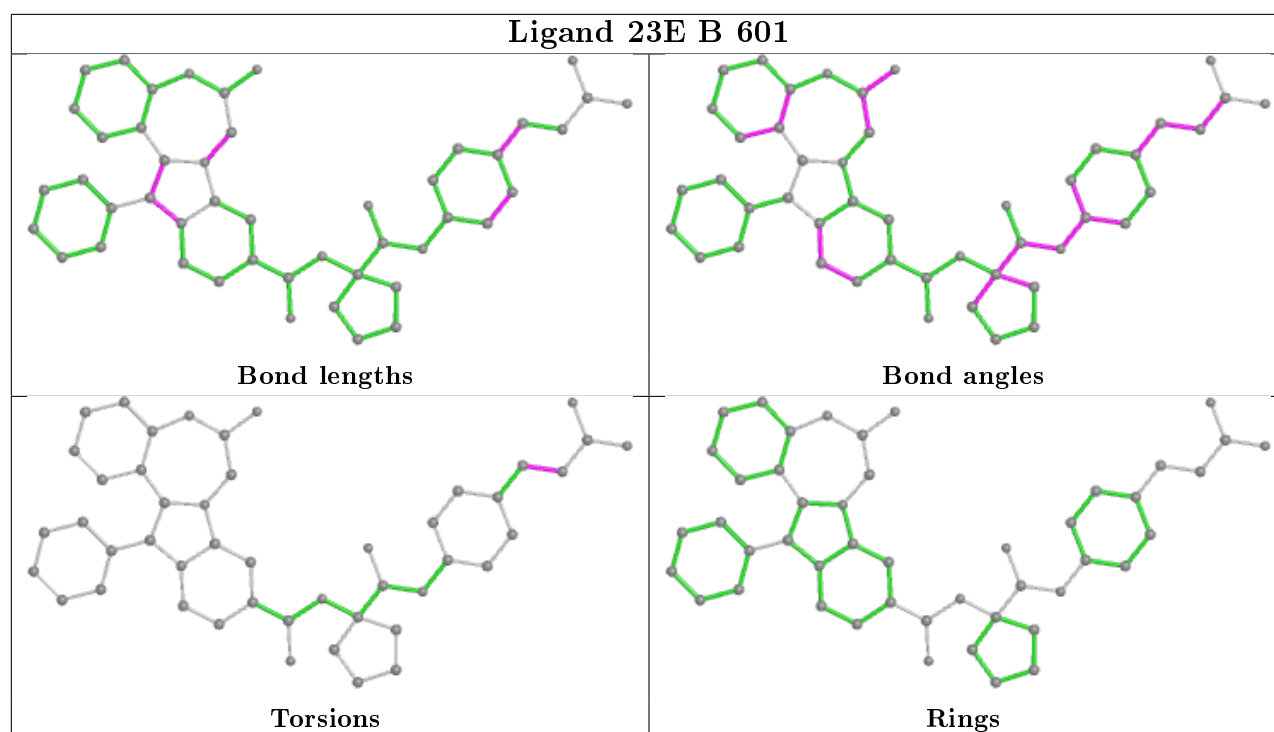
## Ligand 26S B 602



## Ligand 23E A 601







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	538/574 (93%)	0.27	30 (5%) 24 19	22, 38, 78, 134	0
1	B	515/574 (89%)	0.46	54 (10%) 6 4	23, 42, 93, 142	0
All	All	1053/1148 (91%)	0.36	84 (7%) 12 9	22, 40, 84, 142	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	PRO	10.7
1	B	149	PRO	10.4
1	B	150	GLU	10.0
1	A	152	GLY	10.0
1	B	14	CYS	9.7
1	A	154	ARG	9.4
1	A	150	GLU	8.8
1	B	152	GLY	8.4
1	B	153	GLY	8.1
1	A	151	LYS	7.8
1	A	153	GLY	7.8
1	A	13	PRO	6.8
1	A	12	THR	6.7
1	A	148	GLN	6.0
1	A	147	VAL	5.7
1	B	148	GLN	5.5
1	B	154	ARG	5.5
1	B	151	LYS	5.3
1	B	13	PRO	5.1
1	B	402	HIS	5.1
1	B	540	PRO	5.1
1	A	402	HIS	5.0
1	B	110	ASN	4.6
1	B	541	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	47	LEU	4.3
1	A	448	TYR	4.2
1	B	46	SER	4.2
1	B	42	SER	4.2
1	B	147	VAL	4.0
1	B	43	ARG	4.0
1	A	44	SER	4.0
1	B	155	LYS	4.0
1	A	327	ALA	3.8
1	B	146	CYS	3.8
1	B	94	PRO	3.7
1	B	156	PRO	3.7
1	B	45	ALA	3.7
1	A	337	ARG	3.6
1	A	14	CYS	3.5
1	A	43	ARG	3.5
1	A	270	LYS	3.5
1	A	334	ALA	3.4
1	B	7	THR	3.3
1	B	44	SER	3.3
1	A	532	THR	3.2
1	B	404	PRO	3.2
1	B	12	THR	3.1
1	B	50	LYS	3.1
1	B	102	GLY	3.0
1	A	330	GLN	3.0
1	B	113	SER	3.0
1	B	142	ASN	2.9
1	A	46	SER	2.9
1	B	397	TRP	2.9
1	A	331	GLU	2.8
1	B	535	LYS	2.8
1	B	143	GLU	2.8
1	B	401	ARG	2.8
1	A	146	CYS	2.8
1	B	108	VAL	2.7
1	B	9	ALA	2.7
1	B	106	LYS	2.7
1	B	542	ALA	2.7
1	B	96	SER	2.7
1	A	10	LEU	2.6
1	B	95	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	111	LEU	2.5
1	B	269	SER	2.5
1	B	10	LEU	2.4
1	B	107	ASP	2.4
1	A	107	ASP	2.3
1	A	8	GLY	2.3
1	A	106	LYS	2.3
1	B	270	LYS	2.3
1	B	539	ILE	2.2
1	B	103	TYR	2.2
1	B	112	SER	2.2
1	B	101	PHE	2.2
1	B	6	TRP	2.2
1	B	48	ARG	2.2
1	B	399	THR	2.1
1	B	114	LYS	2.1
1	A	449	GLY	2.1
1	B	212	LYS	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	SO4	B	658	5/5	0.75	0.32	123,128,128,129	0
3	SO4	A	652	5/5	0.89	0.19	85,89,90,91	0
3	SO4	B	657	5/5	0.90	0.19	96,100,101,102	0
3	SO4	B	653	5/5	0.92	0.17	83,87,89,89	0
2	23E	B	601	47/47	0.93	0.17	25,37,47,59	0

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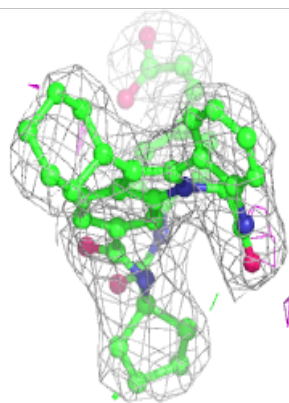
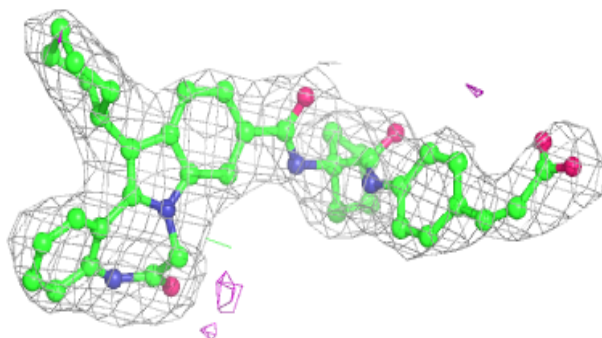
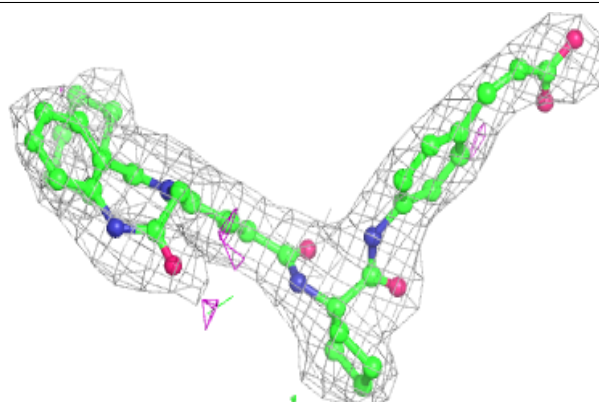
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	23E	A	601	47/47	0.94	0.16	21,31,54,67	0
4	26S	B	602	39/39	0.94	0.15	33,40,50,52	0
3	SO4	B	656	5/5	0.95	0.17	71,75,76,76	0
3	SO4	A	653	5/5	0.95	0.15	53,57,57,58	0

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.

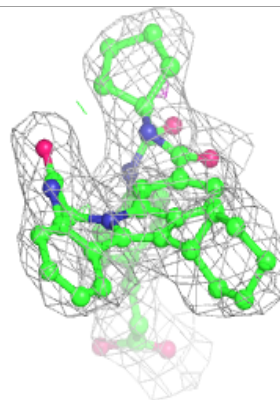
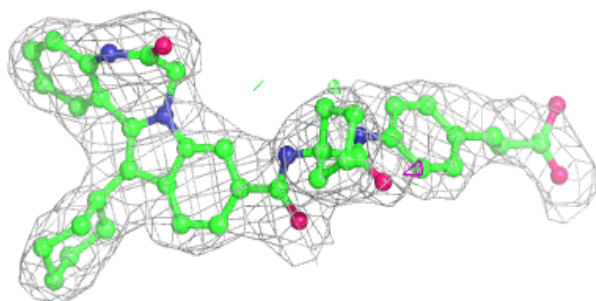
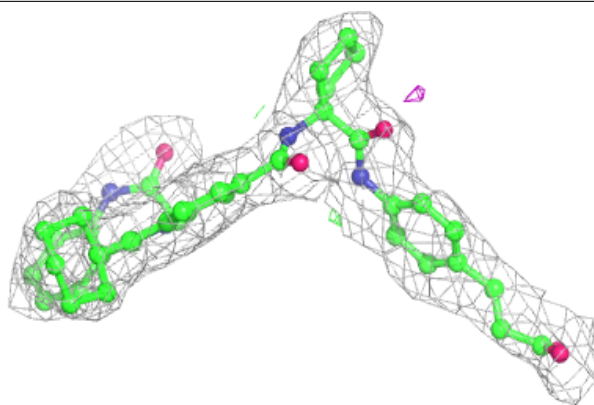
**Electron density around 23E B 601:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



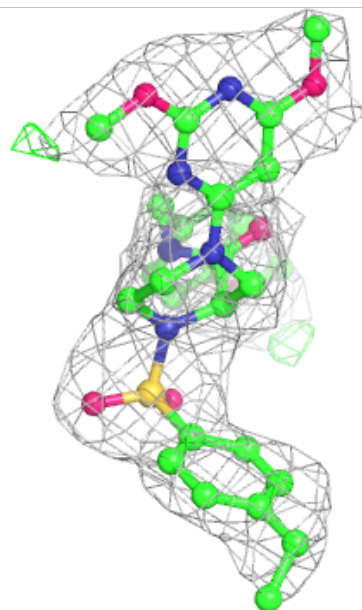
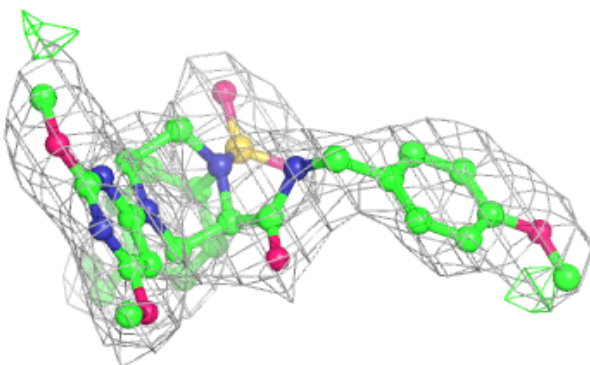
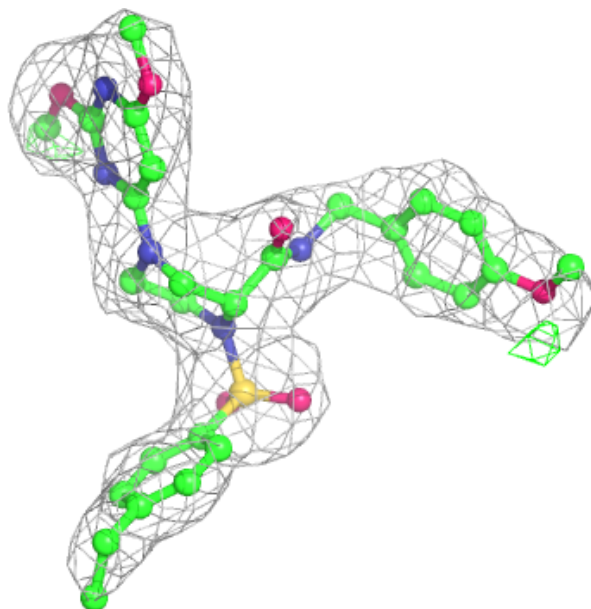
**Electron density around 23E A 601:**

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



**Electron density around 26S B 602:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.