



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:24 AM UTC

PDB ID : 3QGF / pdb_00003qgf
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-(6-chloropyridazin-3-yl)-N-(4-methoxybenzyl)-1-{{4-(trifluoromethoxy)phenyl}sulfonyl}piperazine-2-carboxamide
Authors : Sheriff, S.
Deposited on : 2011-01-24
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

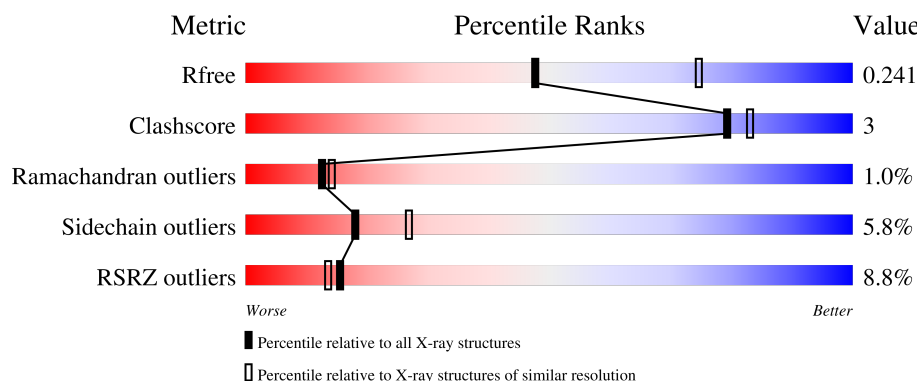
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

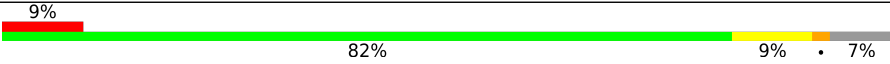
The reported resolution of this entry is 2.45 Å.

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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	574	
1	B	574	

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8753 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.

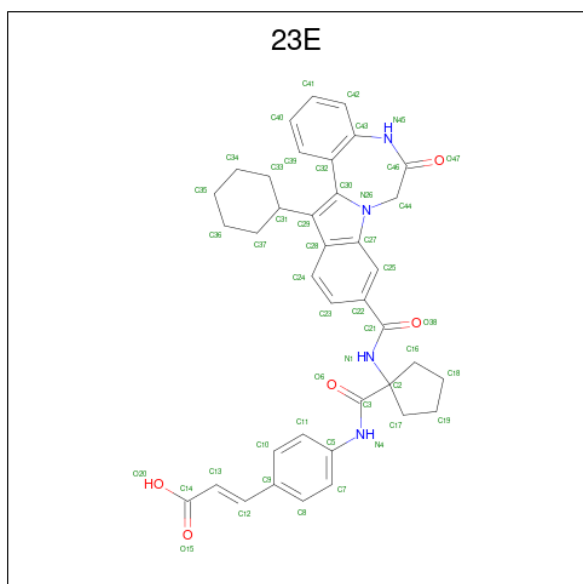
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4145	2613	733	767	32			
1	B	533	Total	C	N	O	S	0	0	0
			4134	2605	731	766	32			

There are 2 discrepancies between the modelled and reference sequences:

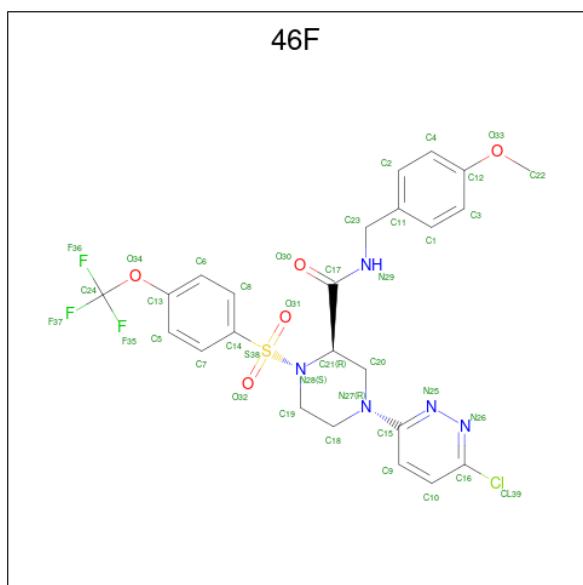
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q9WMX2
B	0	MET	-	initiating methionine	UNP Q9WMX2

- 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 (CCD ID: 23E) (formula: C₃₈H₃₈N₄O₅).



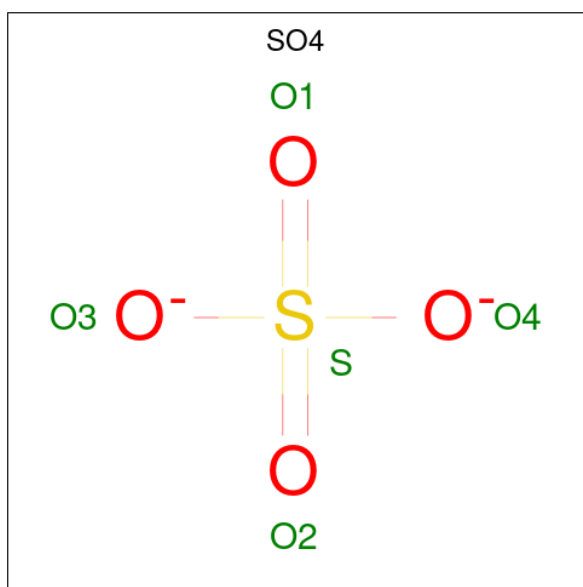
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			47	38	4	5		
2	B	1	Total	C	N	O	0	0
			47	38	4	5		

- Molecule 3 is (2R)-4-(6-chloropyridazin-3-yl)-N-(4-methoxybenzyl)-1-{[4-(trifluoromethoxy)phenyl]sulfonyl}piperazine-2-carboxamide (CCD ID: 46F) (formula: C₂₄H₂₃ClF₃N₅O₅S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	S	0	0
			39	24	1	3	5	5	1		
3	B	1	Total	C	Cl	F	N	O	S	0	0
			39	24	1	3	5	5	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

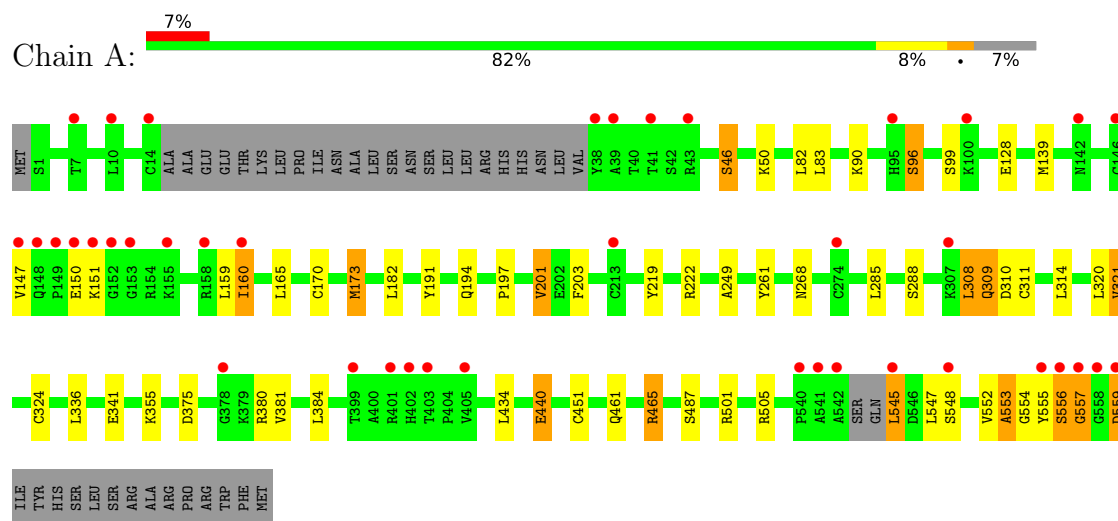
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	129	Total	O	0	0
			129	129		
5	B	123	Total	O	0	0
			123	123		

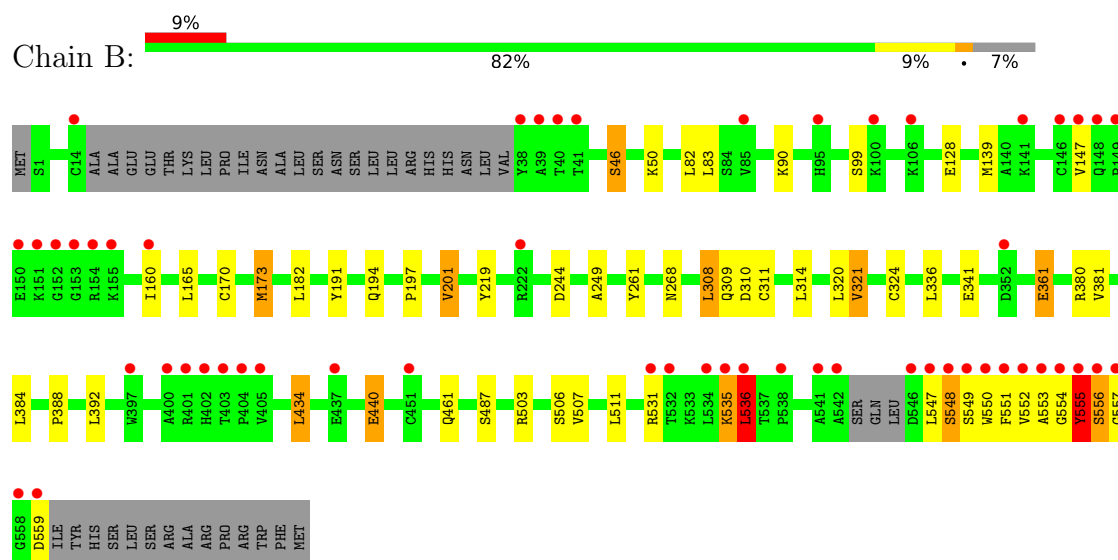
3 Residue-property plots [i](#)

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: 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, α , β , γ	74.90Å 90.10Å 231.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.44 – 2.45 35.44 – 2.45	Depositor EDS
% Data completeness (in resolution range)	85.0 (35.44-2.45) 84.9 (35.44-2.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 2.45Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.9.7, BUSTER 2.9.7	Depositor
R, R_{free}	0.225 , 0.269 (Not available) , 0.241	Depositor DCC
R_{free} test set	1072 reflections (2.14%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8753	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: 46F, SO4, 23E

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	0.85	1/4233 (0.0%)	1.31	11/5740 (0.2%)
1	B	0.84	1/4222 (0.0%)	1.31	13/5726 (0.2%)
All	All	0.84	2/8455 (0.0%)	1.31	24/11466 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	173	MET	SD-CE	-8.16	1.59	1.79
1	A	173	MET	SD-CE	-7.99	1.59	1.79

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	535	LYS	CA-C-N	7.31	134.85	121.70
1	B	535	LYS	C-N-CA	7.31	134.85	121.70
1	A	554	GLY	CA-C-N	7.08	135.07	121.54
1	A	554	GLY	C-N-CA	7.08	135.07	121.54
1	B	548	SER	CA-C-N	6.75	133.86	121.70
1	B	548	SER	C-N-CA	6.75	133.86	121.70
1	A	553	ALA	N-CA-C	6.22	124.05	110.80
1	A	310	ASP	CA-CB-CG	6.21	118.81	112.60
1	B	310	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	201	VAL	N-CA-CB	6.05	118.76	110.54
1	A	548	SER	CA-C-N	5.95	132.90	121.54
1	A	548	SER	C-N-CA	5.95	132.90	121.54
1	B	201	VAL	N-CA-CB	5.94	118.61	110.54
1	B	261	TYR	N-CA-C	5.92	117.73	111.28
1	B	361	GLU	CB-CG-CD	5.91	122.65	112.60
1	A	261	TYR	N-CA-C	5.79	117.58	111.28
1	B	128	GLU	CB-CG-CD	5.74	122.36	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	GLU	CB-CG-CD	5.55	122.04	112.60
1	B	244	ASP	N-CA-C	-5.49	100.85	109.25
1	A	268	ASN	CA-CB-CG	5.25	117.85	112.60
1	B	555	TYR	CA-C-N	5.24	131.56	121.54
1	B	555	TYR	C-N-CA	5.24	131.56	121.54
1	A	375	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	268	ASN	CA-CB-CG	5.00	117.60	112.60

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	4145	0	4162	21	0
1	B	4134	0	4142	23	0
2	A	47	0	37	1	0
2	B	47	0	37	0	0
3	A	39	0	23	1	0
3	B	39	0	23	1	0
4	A	30	0	0	0	0
4	B	20	0	0	0	0
5	A	129	0	0	0	0
5	B	123	0	0	0	0
All	All	8753	0	8424	45	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 (45) 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:A:465:ARG:HG3	1:A:545:LEU:HB3	1.69	0.74
1:B:535:LYS:HA	1:B:536:LEU:HB2	1.69	0.73
1:B:308:LEU:HB3	1:B:311:CYS:SG	2.30	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:HB3	1:A:311:CYS:SG	2.31	0.69
2:A:601:23E:O6	2:A:601:23E:H7	2.02	0.59
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.89	0.55
1:A:288:SER:CB	1:A:556:SER:HB3	2.37	0.55
1:B:83:LEU:HB2	1:B:173:MET:HA	1.89	0.55
1:A:83:LEU:HB2	1:A:173:MET:HA	1.91	0.53
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.91	0.52
1:A:285:LEU:HD12	1:A:557:GLY:HA3	1.92	0.51
1:B:535:LYS:CA	1:B:536:LEU:HB2	2.36	0.51
1:B:434:LEU:HD11	1:B:511:LEU:HG	1.92	0.51
1:B:554:GLY:O	1:B:555:TYR:HB2	2.11	0.51
1:B:197:PRO:HA	3:B:602:46F:H3	1.93	0.51
1:A:288:SER:HB3	1:A:556:SER:HB3	1.95	0.48
1:B:314:LEU:HB3	1:B:321:VAL:HG23	1.95	0.48
1:A:139:MET:HB3	1:A:160:ILE:HG23	1.95	0.48
1:A:197:PRO:HA	3:A:602:46F:H3	1.95	0.48
1:B:556:SER:N	1:B:557:GLY:HA2	2.28	0.47
1:A:314:LEU:HB3	1:A:321:VAL:HG23	1.96	0.47
1:B:503:ARG:O	1:B:507:VAL:HG23	2.15	0.47
1:B:139:MET:HB3	1:B:160:ILE:HG23	1.96	0.47
1:A:309:GLN:O	1:A:324:CYS:HB2	2.15	0.46
1:B:309:GLN:O	1:B:324:CYS:HB2	2.14	0.46
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.98	0.45
1:B:191:TYR:O	1:B:194:GLN:HG2	2.18	0.44
1:B:170:CYS:HA	1:B:173:MET:HE3	2.00	0.44
1:A:191:TYR:O	1:A:194:GLN:HG2	2.18	0.43
1:A:440:GLU:H	1:A:440:GLU:CD	2.25	0.43
1:A:46:SER:O	1:A:50:LYS:HG2	2.19	0.43
1:A:82:LEU:HD13	1:A:249:ALA:HB2	2.00	0.43
1:A:99:SER:HB2	1:A:165:LEU:HB3	2.01	0.43
1:B:548:SER:HB2	1:B:551:PHE:HB2	2.00	0.42
1:A:451:CYS:HB2	1:A:552:VAL:O	2.19	0.42
1:B:440:GLU:H	1:B:440:GLU:CD	2.26	0.42
1:B:99:SER:HB2	1:B:165:LEU:HB3	2.02	0.42
1:B:46:SER:O	1:B:50:LYS:HG2	2.19	0.42
1:A:170:CYS:HA	1:A:173:MET:HE3	2.02	0.42
1:A:501:ARG:O	1:A:505:ARG:HG3	2.21	0.41
1:B:536:LEU:HD22	1:B:536:LEU:HA	1.88	0.41
1:A:96:SER:HA	1:A:559:ASP:C	2.46	0.41
1:A:203:PHE:CE2	1:A:314:LEU:HD13	2.56	0.41
1:B:548:SER:HA	1:B:550:TRP:H	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:PRO:O	1:B:392:LEU:HG	2.21	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	528/574 (92%)	511 (97%)	13 (2%)	4 (1%)	16	20
1	B	527/574 (92%)	507 (96%)	13 (2%)	7 (1%)	9	9
All	All	1055/1148 (92%)	1018 (96%)	26 (2%)	11 (1%)	12	14

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	VAL
1	A	555	TYR
1	B	147	VAL
1	B	536	LEU
1	B	555	TYR
1	B	556	SER
1	A	553	ALA
1	A	557	GLY
1	B	549	SER
1	B	552	VAL
1	B	553	ALA

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	449/486 (92%)	421 (94%)	28 (6%)	16	23
1	B	412/486 (85%)	390 (95%)	22 (5%)	20	30
All	All	861/972 (89%)	811 (94%)	50 (6%)	18	27

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	SER
1	A	90	LYS
1	A	96	SER
1	A	150	GLU
1	A	151	LYS
1	A	159	LEU
1	A	160	ILE
1	A	182	LEU
1	A	201	VAL
1	A	222	ARG
1	A	308	LEU
1	A	309	GLN
1	A	321	VAL
1	A	336	LEU
1	A	341	GLU
1	A	355	LYS
1	A	380	ARG
1	A	381	VAL
1	A	384	LEU
1	A	434	LEU
1	A	440	GLU
1	A	461	GLN
1	A	465	ARG
1	A	487	SER
1	A	545	LEU
1	A	547	LEU
1	A	556	SER
1	A	559	ASP
1	B	46	SER
1	B	90	LYS
1	B	182	LEU
1	B	201	VAL
1	B	308	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	321	VAL
1	B	336	LEU
1	B	341	GLU
1	B	361	GLU
1	B	380	ARG
1	B	381	VAL
1	B	384	LEU
1	B	434	LEU
1	B	440	GLU
1	B	461	GLN
1	B	487	SER
1	B	506	SER
1	B	531	ARG
1	B	536	LEU
1	B	547	LEU
1	B	555	TYR
1	B	559	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	330	GLN
1	A	436	GLN
1	A	514	GLN
1	B	436	GLN
1	B	514	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 oligosaccharides in this entry.

5.6 Ligand geometry

14 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$
4	SO4	B	651	-	4,4,4	0.30	0	6,6,6	0.11	0
4	SO4	B	652	-	4,4,4	0.55	0	6,6,6	0.26	0
4	SO4	A	660	-	4,4,4	0.36	0	6,6,6	0.24	0
3	46F	B	602	-	42,42,42	1.55	4 (9%)	58,61,61	1.87	11 (18%)
4	SO4	A	653	-	4,4,4	0.22	0	6,6,6	0.42	0
4	SO4	B	653	-	4,4,4	0.30	0	6,6,6	0.13	0
4	SO4	A	659	-	4,4,4	0.35	0	6,6,6	0.40	0
2	23E	A	601	-	52,53,53	1.60	7 (13%)	68,77,77	1.21	7 (10%)
4	SO4	B	657	-	4,4,4	0.33	0	6,6,6	0.15	0
2	23E	B	601	-	52,53,53	1.57	6 (11%)	68,77,77	1.16	7 (10%)
3	46F	A	602	-	42,42,42	1.48	2 (4%)	58,61,61	2.04	16 (27%)
4	SO4	A	652	-	4,4,4	0.42	0	6,6,6	0.13	0
4	SO4	A	651	-	4,4,4	0.33	0	6,6,6	0.17	0
4	SO4	A	654	-	4,4,4	0.27	0	6,6,6	0.04	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
3	46F	A	602	-	-	2/32/45/45	0/4/4/4
3	46F	B	602	-	-	2/32/45/45	0/4/4/4
2	23E	B	601	-	-	4/28/57/57	0/6/7/7
2	23E	A	601	-	-	4/28/57/57	0/6/7/7

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	46F	S38-N28	6.36	1.72	1.63
3	A	602	46F	S38-N28	5.64	1.71	1.63
2	A	601	23E	O15-C14	5.02	1.35	1.23
2	B	601	23E	O15-C14	4.71	1.34	1.23
2	B	601	23E	C30-N26	-4.69	1.32	1.39
2	A	601	23E	C30-N26	-4.48	1.32	1.39
2	A	601	23E	C32-C30	4.45	1.51	1.47
2	B	601	23E	C32-C30	4.36	1.51	1.47
2	A	601	23E	C28-C29	3.68	1.50	1.44
2	B	601	23E	C28-C29	3.32	1.49	1.44
3	A	602	46F	C17-N29	3.00	1.40	1.33
3	B	602	46F	O31-S38	3.00	1.46	1.43
3	B	602	46F	C17-N29	2.86	1.40	1.33
2	A	601	23E	O20-C14	-2.76	1.23	1.30
2	B	601	23E	O20-C14	-2.68	1.23	1.30
2	B	601	23E	C27-N26	-2.36	1.35	1.39
2	A	601	23E	C16-C2	2.28	1.57	1.54
2	A	601	23E	C2-C3	-2.11	1.49	1.53
3	B	602	46F	C20-C21	2.02	1.55	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	46F	C21-C20-N27	-7.86	97.54	109.36
3	B	602	46F	C21-C20-N27	-6.99	98.84	109.36
3	B	602	46F	CL39-C16-N26	-4.63	111.77	115.20
3	A	602	46F	CL39-C16-N26	-4.55	111.83	115.20
3	B	602	46F	C19-C18-N27	-4.44	101.45	110.78
3	B	602	46F	C23-N29-C17	4.11	127.94	122.29
2	B	601	23E	C27-C28-C29	-3.91	103.72	107.02
3	A	602	46F	C9-C15-N25	-3.81	118.26	123.84
3	A	602	46F	C19-C18-N27	-3.75	102.89	110.78
3	A	602	46F	C8-C14-S38	-3.56	116.20	119.73
3	A	602	46F	O32-S38-C14	-3.40	103.88	108.10
2	A	601	23E	C27-C28-C29	-3.28	104.26	107.02
3	A	602	46F	C17-C21-N28	-3.11	103.70	111.19
3	A	602	46F	C19-N28-C21	3.10	122.86	114.89
3	A	602	46F	C21-N28-S38	-3.05	111.76	119.33
3	B	602	46F	C18-C19-N28	3.02	112.30	109.00
3	A	602	46F	C10-C16-CL39	2.97	125.32	119.18
2	B	601	23E	C27-N26-C30	2.92	110.71	108.37
3	B	602	46F	C9-C15-N25	-2.86	119.66	123.84
2	B	601	23E	C24-C28-C27	2.81	122.48	119.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	23E	C24-C28-C27	2.74	122.40	119.24
3	B	602	46F	O32-S38-C14	-2.73	104.71	108.10
3	A	602	46F	C15-N25-N26	2.67	121.66	118.97
2	A	601	23E	O6-C3-C2	-2.65	117.03	120.99
3	B	602	46F	C10-C16-CL39	2.56	124.47	119.18
3	B	602	46F	C19-N28-C21	2.46	121.22	114.89
2	A	601	23E	C23-C24-C28	-2.42	116.86	120.86
2	B	601	23E	C28-C29-C31	-2.33	121.08	126.87
3	B	602	46F	C11-C23-N29	-2.31	108.21	113.07
3	B	602	46F	C15-N25-N26	2.27	121.25	118.97
2	A	601	23E	C28-C29-C30	-2.18	105.17	107.28
2	B	601	23E	C23-C24-C28	-2.17	117.28	120.86
2	A	601	23E	C28-C29-C31	-2.13	121.56	126.87
3	A	602	46F	C10-C9-C15	2.11	120.58	117.65
3	A	602	46F	O32-S38-O31	2.11	122.88	119.59
3	A	602	46F	C10-C16-N26	-2.10	122.85	124.68
3	A	602	46F	C8-C14-C7	2.07	123.17	120.47
3	A	602	46F	C5-C7-C14	-2.04	117.46	119.44
2	B	601	23E	C35-C34-C33	-2.02	107.27	111.42
2	B	601	23E	C16-C2-C3	2.02	115.46	110.75
2	A	601	23E	C17-C2-C3	-2.01	106.06	110.75

There are no chirality outliers.

All (12) torsion outliers are listed below:

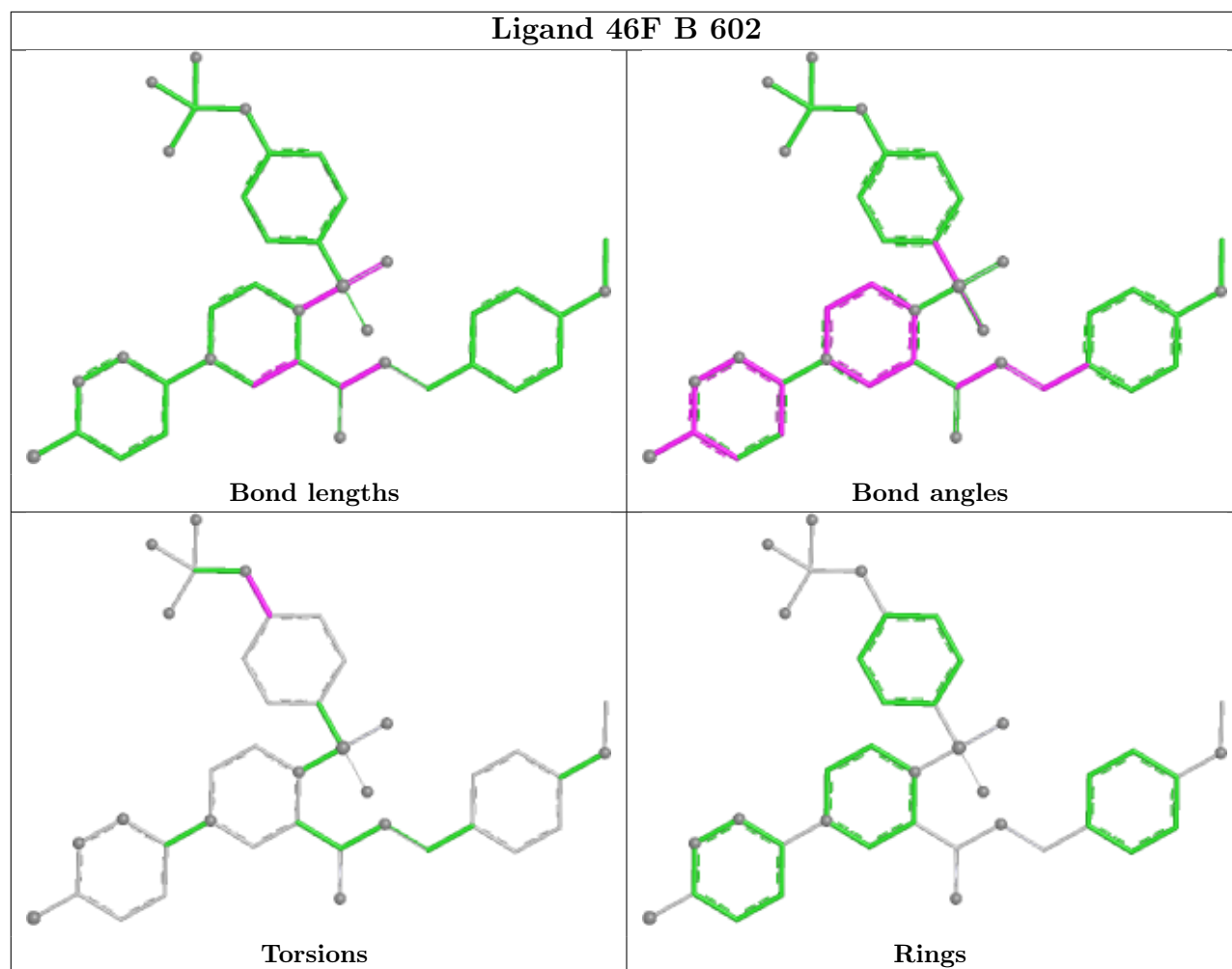
Mol	Chain	Res	Type	Atoms
2	B	601	23E	C12-C13-C14-O15
2	B	601	23E	C12-C13-C14-O20
2	A	601	23E	C12-C13-C14-O15
2	A	601	23E	C12-C13-C14-O20
2	A	601	23E	C13-C12-C9-C8
2	B	601	23E	C17-C2-C3-O6
2	A	601	23E	C13-C12-C9-C10
3	A	602	46F	C5-C13-O34-C24
2	B	601	23E	C16-C2-C3-O6
3	A	602	46F	C6-C13-O34-C24
3	B	602	46F	C6-C13-O34-C24
3	B	602	46F	C5-C13-O34-C24

There are no ring outliers.

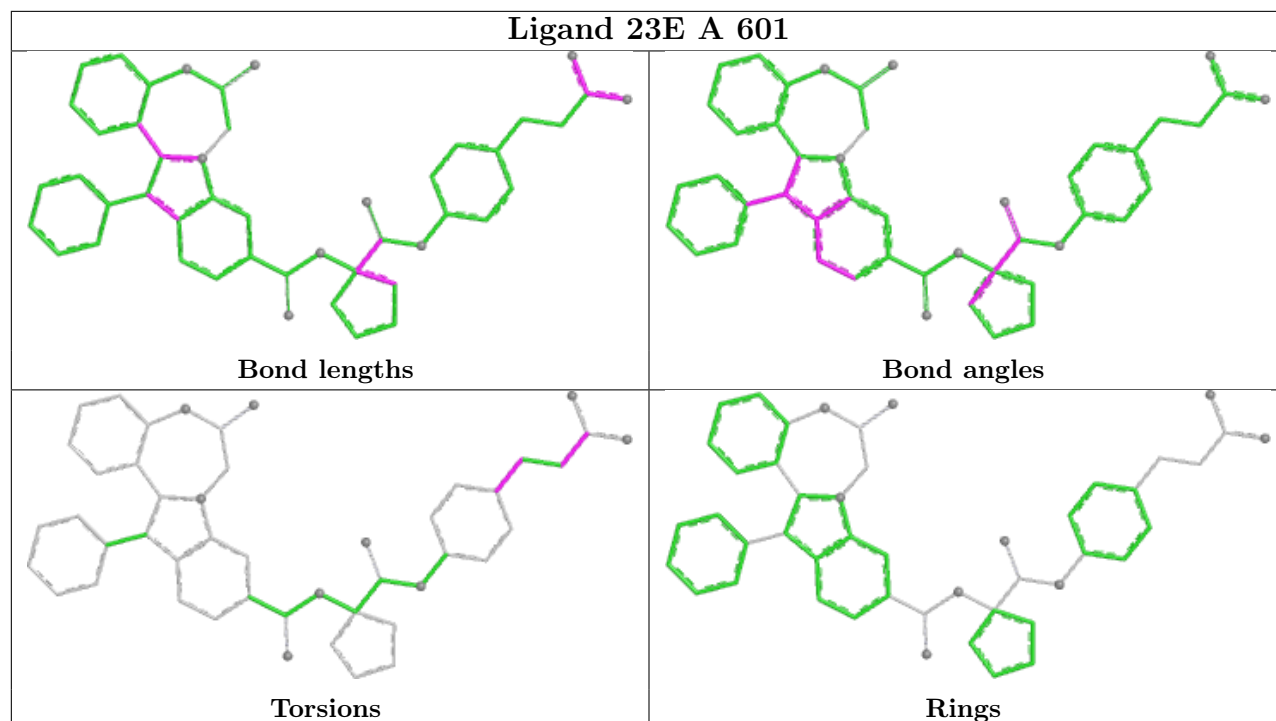
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	46F	1	0
2	A	601	23E	1	0
3	A	602	46F	1	0

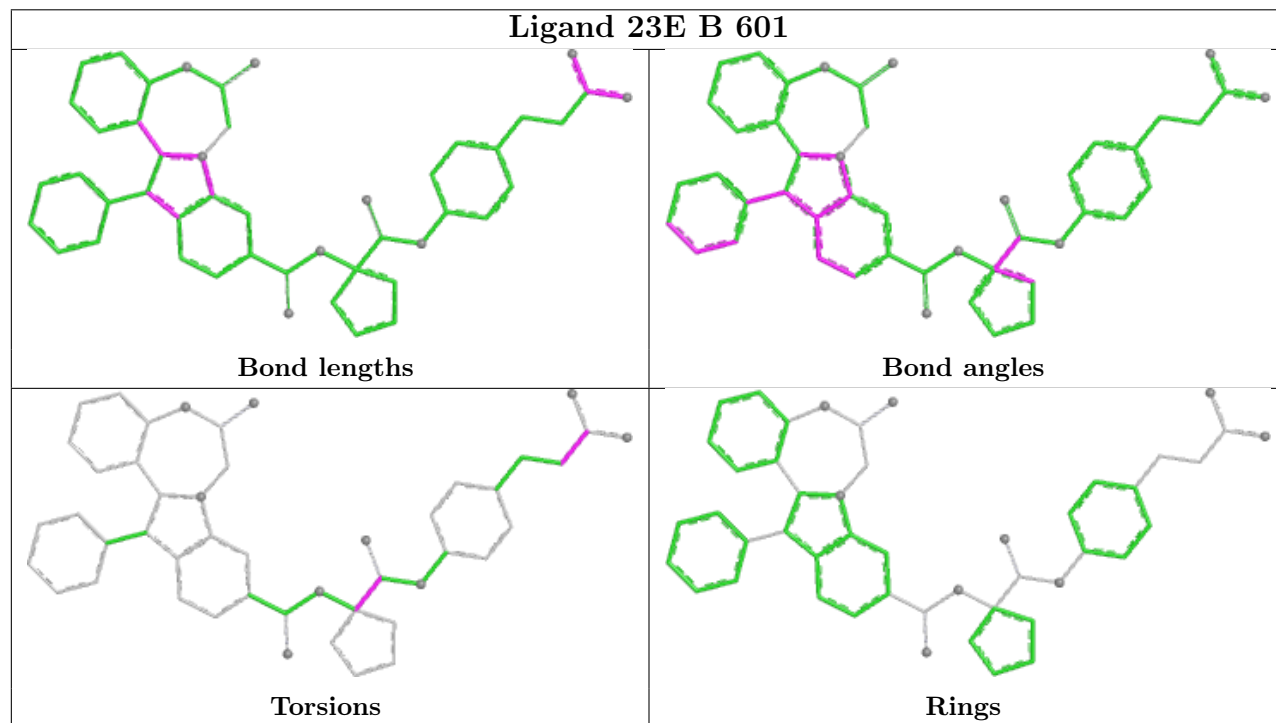
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

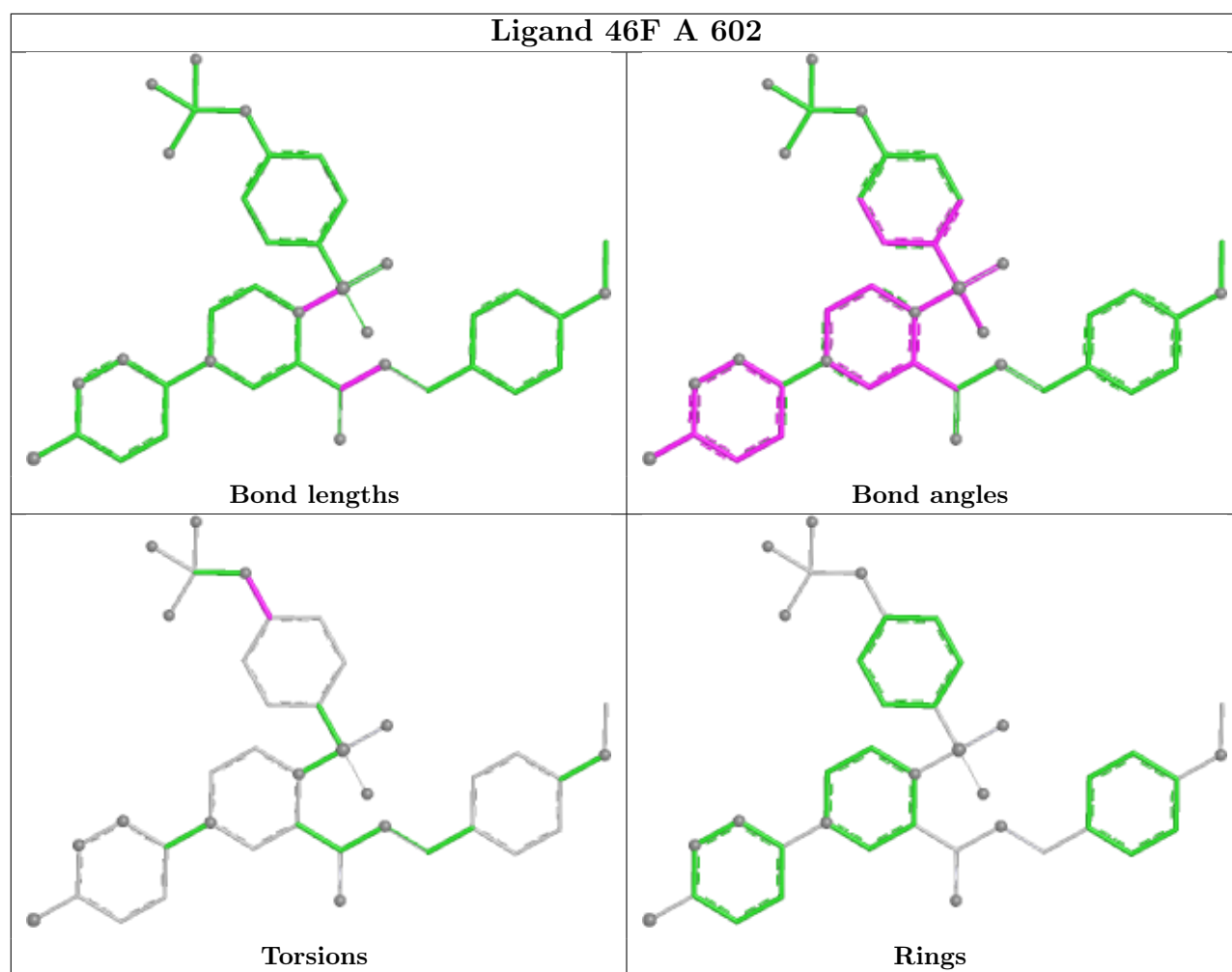


Ligand 23E A 601



Ligand 23E B 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, 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	534/574 (93%)	0.33	40 (7%)	20	17	10, 27, 59, 115	0
1	B	533/574 (92%)	0.55	54 (10%)	12	10	12, 31, 76, 114	0
All	All	1067/1148 (92%)	0.44	94 (8%)	15	13	10, 29, 68, 115	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	556	SER	8.5
1	A	147	VAL	7.6
1	B	147	VAL	7.6
1	B	402	HIS	7.4
1	B	148	GLN	7.0
1	A	148	GLN	6.6
1	B	557	GLY	6.3
1	B	542	ALA	6.3
1	A	149	PRO	6.2
1	B	149	PRO	5.8
1	A	559	ASP	5.7
1	B	14	CYS	5.7
1	B	555	TYR	5.5
1	A	14	CYS	5.4
1	B	547	LEU	5.4
1	A	557	GLY	5.4
1	B	559	ASP	5.2
1	B	556	SER	5.2
1	A	558	GLY	5.1
1	A	542	ALA	4.8
1	B	558	GLY	4.7
1	B	151	LYS	4.5
1	A	555	TYR	4.5
1	A	151	LYS	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	150	GLU	4.4
1	B	552	VAL	4.3
1	B	153	GLY	4.2
1	B	404	PRO	4.1
1	B	541	ALA	4.1
1	B	550	TRP	3.9
1	A	541	ALA	3.9
1	A	152	GLY	3.7
1	A	545	LEU	3.7
1	B	405	VAL	3.7
1	B	534	LEU	3.7
1	B	437	GLU	3.6
1	B	535	LYS	3.4
1	A	540	PRO	3.4
1	B	549	SER	3.3
1	B	546	ASP	3.3
1	A	402	HIS	3.2
1	A	548	SER	3.2
1	B	100	LYS	3.1
1	B	551	PHE	3.1
1	B	548	SER	3.1
1	A	160	ILE	3.1
1	B	554	GLY	3.0
1	B	141	LYS	3.0
1	B	403	THR	3.0
1	B	553	ALA	3.0
1	A	95	HIS	2.9
1	B	154	ARG	2.8
1	B	160	ILE	2.8
1	A	146	CYS	2.8
1	A	153	GLY	2.7
1	B	152	GLY	2.7
1	B	532	THR	2.7
1	B	146	CYS	2.7
1	A	7	THR	2.7
1	B	38	TYR	2.6
1	B	536	LEU	2.6
1	A	399	THR	2.6
1	A	10	LEU	2.6
1	A	100	LYS	2.5
1	A	213	CYS	2.5
1	B	352	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	538	PRO	2.4
1	A	155	LYS	2.4
1	B	155	LYS	2.4
1	A	158	ARG	2.4
1	A	41	THR	2.4
1	A	401	ARG	2.4
1	B	451	CYS	2.4
1	B	397	TRP	2.4
1	A	38	TYR	2.3
1	A	403	THR	2.3
1	A	378	GLY	2.3
1	B	85	VAL	2.3
1	A	274	CYS	2.3
1	B	531	ARG	2.3
1	B	40	THR	2.3
1	B	106	LYS	2.3
1	B	39	ALA	2.2
1	A	43	ARG	2.2
1	B	222	ARG	2.2
1	B	400	ALA	2.1
1	A	307	LYS	2.1
1	B	95	HIS	2.1
1	A	405	VAL	2.1
1	A	142	ASN	2.1
1	A	39	ALA	2.0
1	B	150	GLU	2.0
1	B	401	ARG	2.0
1	B	41	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,

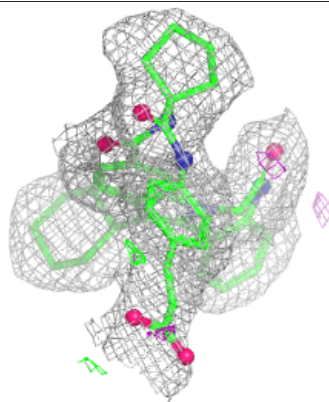
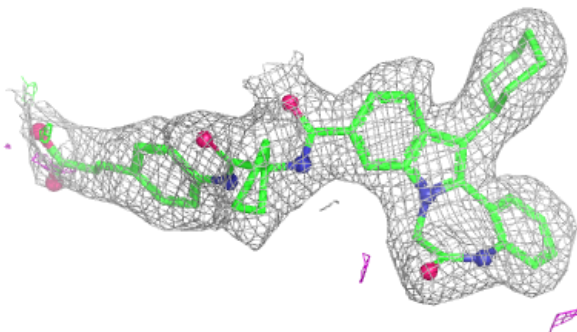
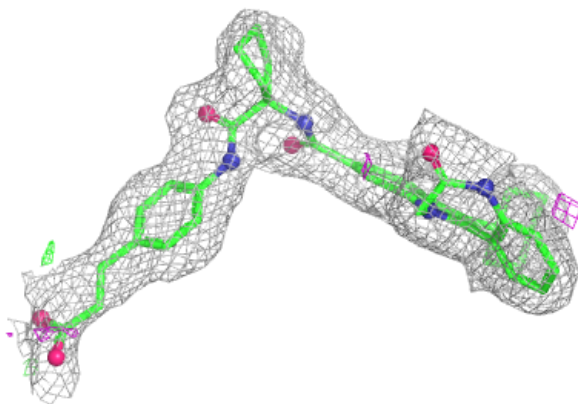
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	B	651	5/5	0.47	0.29	183,188,188,189	0
4	SO4	A	651	5/5	0.66	0.19	121,126,127,127	0
4	SO4	A	654	5/5	0.75	0.24	154,158,159,160	0
4	SO4	A	652	5/5	0.76	0.17	97,102,102,103	0
4	SO4	B	657	5/5	0.77	0.17	117,121,122,123	0
4	SO4	A	660	5/5	0.78	0.20	94,98,99,100	0
4	SO4	B	652	5/5	0.86	0.16	58,61,64,65	0
4	SO4	B	653	5/5	0.91	0.09	62,66,67,68	0
4	SO4	A	659	5/5	0.93	0.09	40,43,45,47	0
2	23E	A	601	47/47	0.93	0.09	12,19,43,55	0
3	46F	B	602	39/39	0.94	0.09	18,31,39,41	0
2	23E	B	601	47/47	0.94	0.08	6,28,48,58	0
3	46F	A	602	39/39	0.96	0.07	12,22,33,35	0
4	SO4	A	653	5/5	0.99	0.05	23,26,30,31	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.

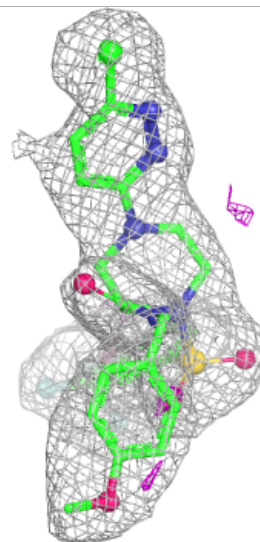
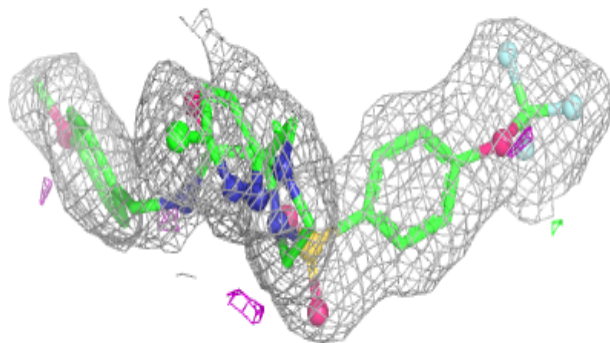
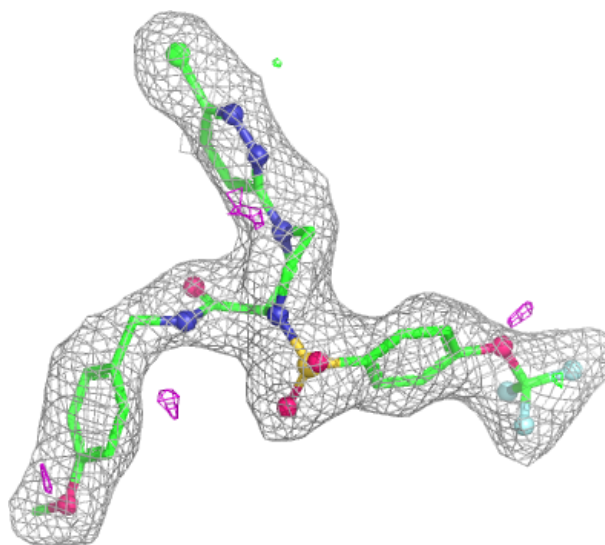
Electron density around 23E A 601:

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



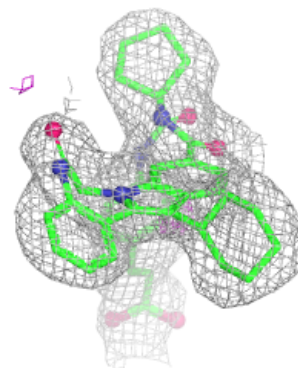
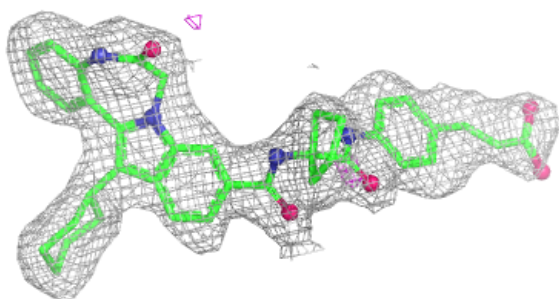
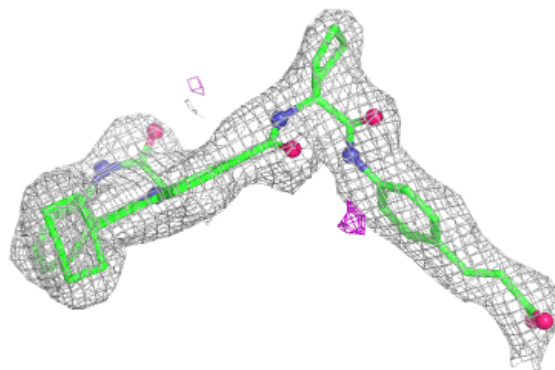
Electron density around 46F B 602:

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



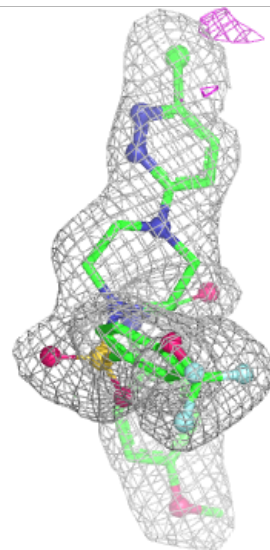
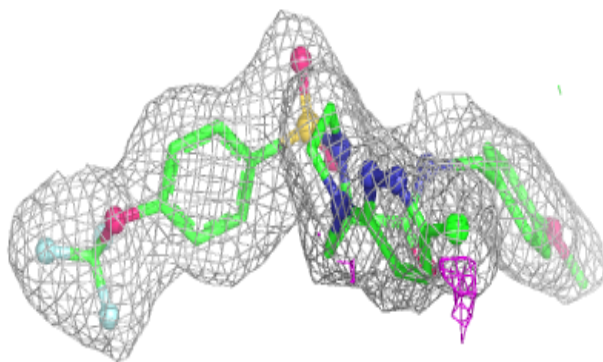
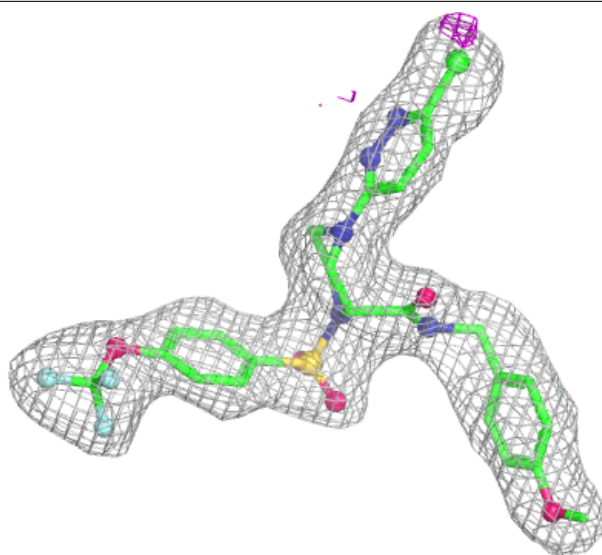
Electron density around 23E B 601:

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



Electron density around 46F A 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 [i](#)

There are no such residues in this entry.