



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:03 AM UTC

PDB ID : 5PZP / pdb_00005pzp
Title : CRYSTAL STRUCTURE OF THE HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE IN COMPLEX WITH 4-FLUORO-2-(4-FLUOROPHENYL)-N-METHYL-5-(2-METHYL-5-{[1-(PYRIMIDIN-2-YL)CYCLOPROPYL]CARBAMOYL}PHENYL)-1-BENZOFURAN-3-CARBOXAMIDE (BMS-929075)
Authors : Sheriff, S.
Deposited on : 2017-02-27
Resolution : 2.95 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)

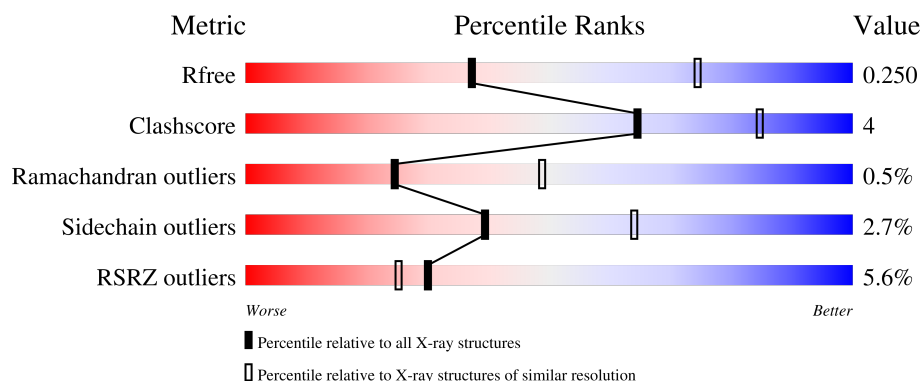
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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 6 unique types of molecules in this entry. The entry contains 8657 atoms, of which 124 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.

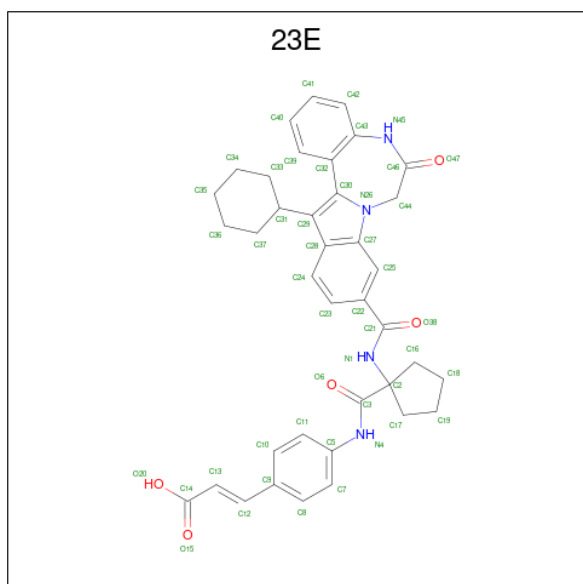
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4205	2653	740	779	33			
1	B	535	Total	C	N	O	S	0	0	0
			4080	2567	717	764	32			

There are 2 discrepancies between the modelled and reference sequences:

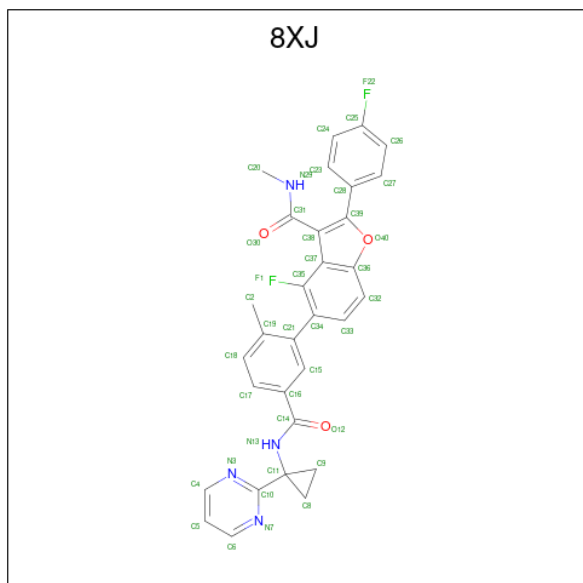
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q9WMX2
B	0	MET	-	expression tag	UNP Q9WMX2

- 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	H	N	O	38	0
			85	38	38	4	5		
2	B	1	Total	C	H	N	O	38	0
			85	38	38	4	5		

- Molecule 3 is 4-fluoro-2-(4-fluorophenyl)-N-methyl-5-(2-methyl-5-{[1-(pyrimidin-2-yl) cyclopropyl]carbamoyl}phenyl)-1-benzofuran-3-carboxamide (CCD ID: 8XJ) (formula: C₃₁H₂₄F₂N₄O₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 64	C 31	F 2	H 24	N 4	O 3	24	0
3	B	1	Total 64	C 31	F 2	H 24	N 4	O 3	24	0

- 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	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 GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

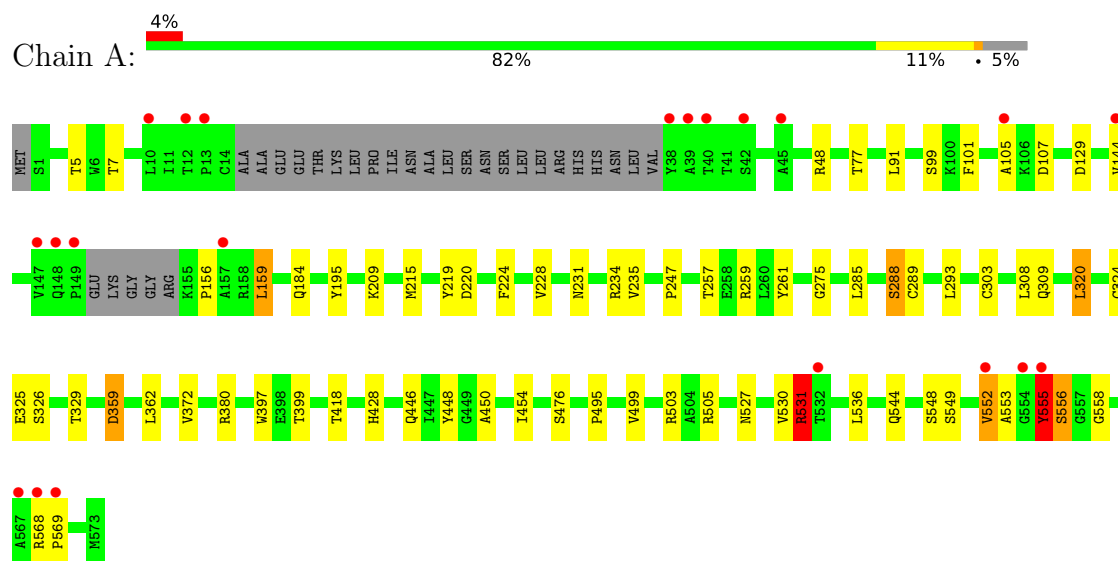
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	1	Total	O	0	0
			1	1		

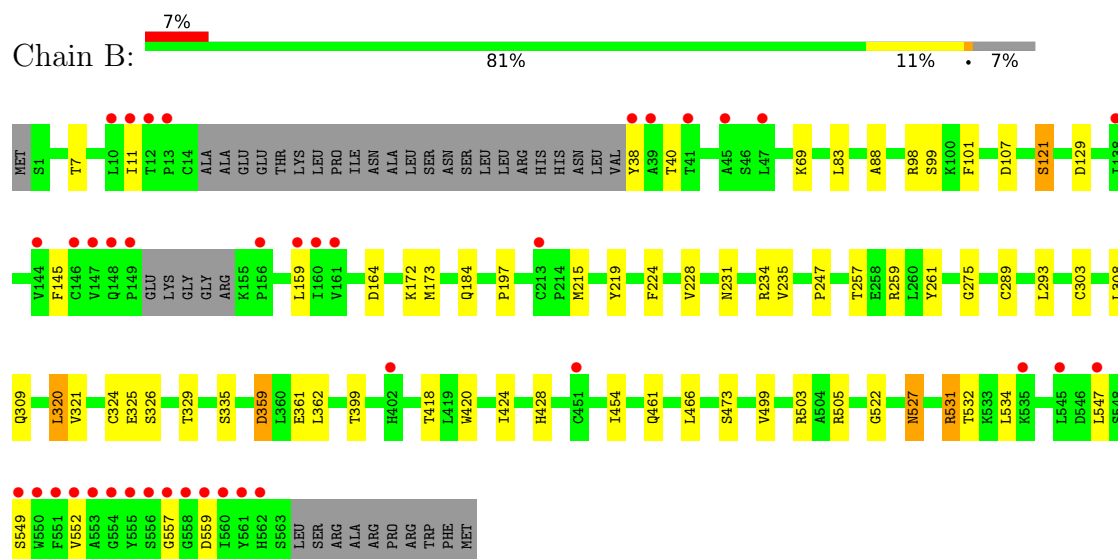
3 Residue-property plots

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	65.20Å 90.70Å 234.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.86 – 2.95 43.86 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.86-2.95) 99.6 (43.86-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.199 , 0.244 0.203 , 0.250	Depositor DCC
R_{free} test set	1057 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8657	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: 8XJ, GOL, 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	0.91	4/4298 (0.1%)	1.33	15/5839 (0.3%)
1	B	0.87	0/4164	1.33	16/5660 (0.3%)
All	All	0.89	4/8462 (0.0%)	1.33	31/11499 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	552	VAL	CA-C	5.40	1.59	1.52
1	A	495	PRO	CA-C	5.35	1.54	1.51
1	A	372	VAL	CA-C	5.25	1.58	1.52
1	A	568	ARG	CA-C	5.17	1.59	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	ASP	CA-C-N	7.41	129.96	120.70
1	B	107	ASP	C-N-CA	7.41	129.96	120.70
1	A	548	SER	CA-C-N	6.27	128.69	120.28
1	A	548	SER	C-N-CA	6.27	128.69	120.28
1	B	359	ASP	CA-CB-CG	6.14	118.74	112.60
1	B	361	GLU	CB-CG-CD	6.05	122.88	112.60
1	A	107	ASP	CA-C-N	5.80	127.94	120.70
1	A	107	ASP	C-N-CA	5.80	127.94	120.70
1	A	359	ASP	CA-CB-CG	5.76	118.36	112.60
1	B	121	SER	CA-C-N	5.63	127.65	120.56
1	B	121	SER	C-N-CA	5.63	127.65	120.56
1	B	418	THR	CA-C-N	5.54	128.01	120.54
1	B	418	THR	C-N-CA	5.54	128.01	120.54
1	A	293	LEU	CA-C-N	5.51	127.60	120.44
1	A	293	LEU	C-N-CA	5.51	127.60	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	289	CYS	CA-C-N	5.38	125.91	119.94
1	B	289	CYS	C-N-CA	5.38	125.91	119.94
1	B	522	GLY	CA-C-N	5.30	127.64	120.65
1	B	522	GLY	C-N-CA	5.30	127.64	120.65
1	A	418	THR	CA-C-N	5.29	127.32	120.44
1	A	418	THR	C-N-CA	5.29	127.32	120.44
1	B	293	LEU	CA-C-N	5.27	127.29	120.44
1	B	293	LEU	C-N-CA	5.27	127.29	120.44
1	B	164	ASP	CA-C-N	5.21	127.27	120.28
1	B	164	ASP	C-N-CA	5.21	127.27	120.28
1	A	289	CYS	CA-C-N	5.21	125.72	119.94
1	A	289	CYS	C-N-CA	5.21	125.72	119.94
1	A	195	TYR	N-CA-C	5.18	117.94	109.59
1	A	555	TYR	N-CA-C	5.14	117.48	110.24
1	A	531	ARG	CA-C-N	5.12	129.50	122.84
1	A	531	ARG	C-N-CA	5.12	129.50	122.84

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	4205	0	4155	37	0
1	B	4080	0	4027	32	0
2	A	47	38	37	0	0
2	B	47	38	37	0	0
3	A	40	24	0	0	0
3	B	40	24	0	0	0
4	A	20	0	0	0	0
4	B	20	0	0	0	0
5	A	18	0	24	1	0
5	B	6	0	8	0	0
6	A	9	0	0	1	0
6	B	1	0	0	1	0
All	All	8533	124	8288	66	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 4.

All (66) 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:309:GLN:HG3	1:A:325:GLU:HB3	1.61	0.81
1:B:309:GLN:HG3	1:B:325:GLU:HB3	1.61	0.80
1:A:359:ASP:HB2	1:A:362:LEU:HD12	1.73	0.69
1:A:505:ARG:HH21	1:A:531:ARG:HG3	1.57	0.68
1:A:288:SER:CB	1:A:555:TYR:HB3	2.23	0.67
1:B:359:ASP:HB2	1:B:362:LEU:HD12	1.78	0.65
1:A:247:PRO:HG3	1:B:234:ARG:HD3	1.79	0.65
1:B:531:ARG:HD3	1:B:532:THR:HG22	1.79	0.64
1:A:448:TYR:O	1:A:556:SER:HA	2.00	0.62
1:A:505:ARG:NH2	1:A:531:ARG:HG3	2.17	0.60
1:B:303:CYS:HA	1:B:308:LEU:HD12	1.89	0.55
1:A:505:ARG:HD3	5:A:609:GOL:H32	1.88	0.55
1:A:288:SER:HB2	1:A:555:TYR:HB3	1.86	0.55
1:A:285:LEU:HA	1:A:558:GLY:HA2	1.88	0.54
1:A:303:CYS:HA	1:A:308:LEU:HD12	1.90	0.54
1:B:531:ARG:HH11	1:B:531:ARG:HG3	1.73	0.53
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.90	0.53
1:A:399:THR:HG21	1:A:428:HIS:NE2	2.23	0.53
1:B:99:SER:C	1:B:101:PHE:H	2.17	0.52
1:A:446:GLN:HA	1:A:450:ALA:O	2.08	0.52
1:B:399:THR:HG21	1:B:428:HIS:NE2	2.24	0.52
1:B:505:ARG:HE	1:B:531:ARG:HH12	1.59	0.49
1:A:184:GLN:HB2	6:A:703:HOH:O	2.12	0.49
1:A:288:SER:HB3	1:A:555:TYR:HB3	1.92	0.49
1:A:231:ASN:O	1:A:235:VAL:HG23	2.12	0.49
1:B:527:ASN:HD21	1:B:534:LEU:HB2	1.77	0.49
1:B:231:ASN:O	1:B:235:VAL:HG23	2.13	0.48
1:A:215:MET:HB2	1:A:326:SER:HB2	1.95	0.48
1:A:499:VAL:O	1:A:503:ARG:HG3	2.13	0.48
1:B:215:MET:HE3	1:B:324:CYS:SG	2.53	0.48
1:A:549:SER:HA	1:A:552:VAL:HG22	1.95	0.47
1:A:553:ALA:HA	1:A:555:TYR:CZ	2.49	0.47
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.95	0.47
1:B:172:LYS:HE2	1:B:559:ASP:O	2.13	0.47
1:A:48:ARG:HG2	1:A:159:LEU:HD13	1.97	0.47
1:B:88:ALA:HB2	1:B:173:MET:HG2	1.97	0.47
1:B:499:VAL:O	1:B:503:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:GLN:HB2	6:B:701:HOH:O	2.15	0.46
1:A:99:SER:C	1:A:101:PHE:H	2.23	0.45
1:A:209:LYS:HZ1	1:A:380:ARG:HH22	1.64	0.45
1:B:531:ARG:HG3	1:B:531:ARG:NH1	2.31	0.45
1:B:215:MET:HB2	1:B:326:SER:HB2	1.98	0.45
1:A:129:ASP:HB3	1:A:259:ARG:NH1	2.32	0.45
1:A:144:VAL:HG21	1:A:397:TRP:CG	2.52	0.45
1:B:7:THR:HG23	1:B:275:GLY:HA2	1.99	0.44
1:A:234:ARG:HD3	1:B:247:PRO:HG3	2.00	0.44
1:B:505:ARG:HE	1:B:531:ARG:NH1	2.15	0.44
1:B:129:ASP:HB3	1:B:259:ARG:NH1	2.33	0.44
1:A:7:THR:HG23	1:A:275:GLY:HA2	1.99	0.43
1:A:224:PHE:O	1:A:228:VAL:HG23	2.18	0.43
1:B:197:PRO:HD2	1:B:466:LEU:HB3	2.01	0.43
1:A:288:SER:HB2	1:A:555:TYR:CB	2.48	0.43
1:A:48:ARG:HB2	1:A:156:PRO:HB2	1.99	0.43
1:A:215:MET:HE3	1:A:324:CYS:SG	2.60	0.42
1:B:224:PHE:O	1:B:228:VAL:HG23	2.19	0.42
1:B:531:ARG:HD2	1:B:532:THR:H	1.84	0.42
1:A:527:ASN:O	1:A:530:VAL:HG22	2.19	0.42
1:B:547:LEU:C	1:B:549:SER:H	2.28	0.42
1:A:77:THR:HA	1:B:69:LYS:HD3	2.02	0.42
1:B:257:THR:HA	1:B:261:TYR:HB2	2.02	0.41
1:B:420:TRP:HA	1:B:424:ILE:HD12	2.01	0.41
1:A:257:THR:HA	1:A:261:TYR:HB2	2.02	0.41
1:B:83:LEU:HB2	1:B:173:MET:HA	2.02	0.41
1:A:5:THR:O	1:A:275:GLY:HA3	2.20	0.41
1:A:544:GLN:OE1	1:A:569:PRO:HA	2.21	0.40
1:B:38:TYR:CE1	1:B:145:PHE:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	539/574 (94%)	511 (95%)	25 (5%)	3 (1%)	21	45
1	B	529/574 (92%)	495 (94%)	32 (6%)	2 (0%)	30	53
All	All	1068/1148 (93%)	1006 (94%)	57 (5%)	5 (0%)	24	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	552	VAL
1	A	105	ALA
1	B	557	GLY
1	A	531	ARG
1	A	556	SER

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	448/486 (92%)	438 (98%)	10 (2%)	45	69
1	B	434/486 (89%)	420 (97%)	14 (3%)	34	59
All	All	882/972 (91%)	858 (97%)	24 (3%)	39	64

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	LEU
1	A	159	LEU
1	A	220	ASP
1	A	288	SER
1	A	320	LEU
1	A	329	THR
1	A	454	ILE
1	A	476	SER
1	A	536	LEU
1	A	555	TYR
1	B	11	ILE

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Mol	Chain	Res	Type
1	B	40	THR
1	B	98	ARG
1	B	121	SER
1	B	159	LEU
1	B	320	LEU
1	B	321	VAL
1	B	329	THR
1	B	335	SER
1	B	454	ILE
1	B	461	GLN
1	B	473	SER
1	B	527	ASN
1	B	531	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	110	ASN
1	A	117	ASN
1	A	142	ASN
1	A	251	GLN
1	A	411	ASN
1	B	110	ASN
1	B	117	ASN
1	B	142	ASN
1	B	194	GLN
1	B	251	GLN
1	B	272	GLN
1	B	406	ASN
1	B	411	ASN
1	B	527	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	23E	A	601	-	52,53,53	0.45	0	68,77,77	0.55	0
2	23E	B	601	-	52,53,53	0.34	0	68,77,77	0.61	1 (1%)
4	SO4	A	606	-	4,4,4	0.33	0	6,6,6	0.38	0
4	SO4	B	603	-	4,4,4	0.37	0	6,6,6	0.16	0
4	SO4	A	603	-	4,4,4	0.27	0	6,6,6	0.14	0
4	SO4	B	604	-	4,4,4	0.43	0	6,6,6	0.39	0
4	SO4	B	606	-	4,4,4	0.42	0	6,6,6	0.31	0
5	GOL	A	607	-	5,5,5	0.11	0	5,5,5	0.19	0
5	GOL	A	609	-	5,5,5	0.13	0	5,5,5	0.23	0
5	GOL	B	607	-	5,5,5	0.09	0	5,5,5	0.24	0
3	8XJ	A	602	-	44,45,45	0.35	0	60,67,67	0.72	2 (3%)
3	8XJ	B	602	-	44,45,45	0.44	0	60,67,67	0.73	1 (1%)
5	GOL	A	608	-	5,5,5	0.19	0	5,5,5	0.29	0
4	SO4	A	604	-	4,4,4	0.34	0	6,6,6	0.29	0
4	SO4	B	605	-	4,4,4	0.50	0	6,6,6	0.34	0
4	SO4	A	605	-	4,4,4	0.42	0	6,6,6	0.22	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	23E	A	601	-	-	4/28/57/57	0/6/7/7
2	23E	B	601	-	-	4/28/57/57	0/6/7/7
5	GOL	A	609	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	607	-	-	2/4/4/4	-
5	GOL	B	607	-	-	0/4/4/4	-
3	8XJ	A	602	-	-	3/23/33/33	0/6/6/6
3	8XJ	B	602	-	-	3/23/33/33	0/6/6/6
5	GOL	A	608	-	-	0/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	8XJ	C9-C11-N13	3.15	119.58	115.21
3	B	602	8XJ	C8-C11-N13	2.74	119.00	115.21
3	A	602	8XJ	C8-C11-N13	2.11	118.13	115.21
2	B	601	23E	C3-C2-N1	2.03	113.61	110.76

There are no chirality outliers.

All (17) torsion outliers are listed below:

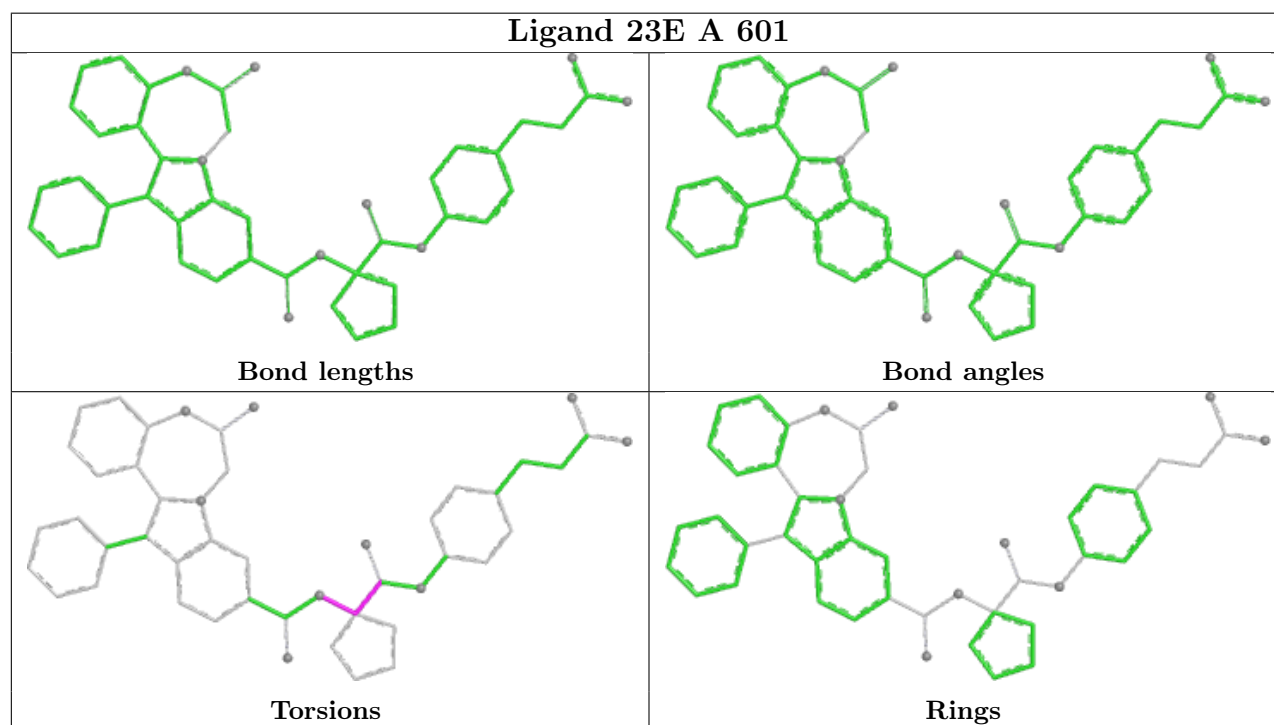
Mol	Chain	Res	Type	Atoms
2	A	601	23E	C3-C2-N1-C21
2	A	601	23E	C16-C2-N1-C21
2	B	601	23E	C3-C2-N1-C21
2	B	601	23E	C16-C2-N1-C21
5	A	607	GOL	C1-C2-C3-O3
2	A	601	23E	C17-C2-N1-C21
5	A	607	GOL	O2-C2-C3-O3
2	B	601	23E	C17-C2-N1-C21
3	A	602	8XJ	O30-C31-C38-C39
5	A	609	GOL	O2-C2-C3-O3
3	B	602	8XJ	C8-C11-N13-C14
3	A	602	8XJ	N29-C31-C38-C39
2	A	601	23E	C17-C2-C3-O6
3	B	602	8XJ	C9-C11-N13-C14
3	A	602	8XJ	N29-C31-C38-C37
2	B	601	23E	C16-C2-C3-O6
3	B	602	8XJ	N29-C31-C38-C39

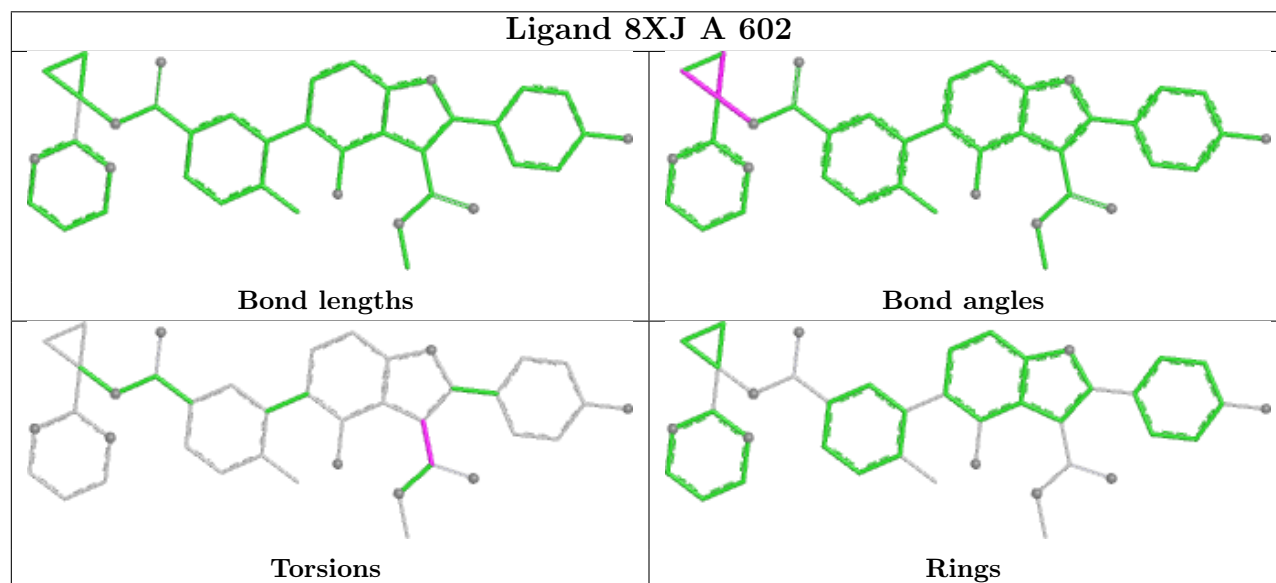
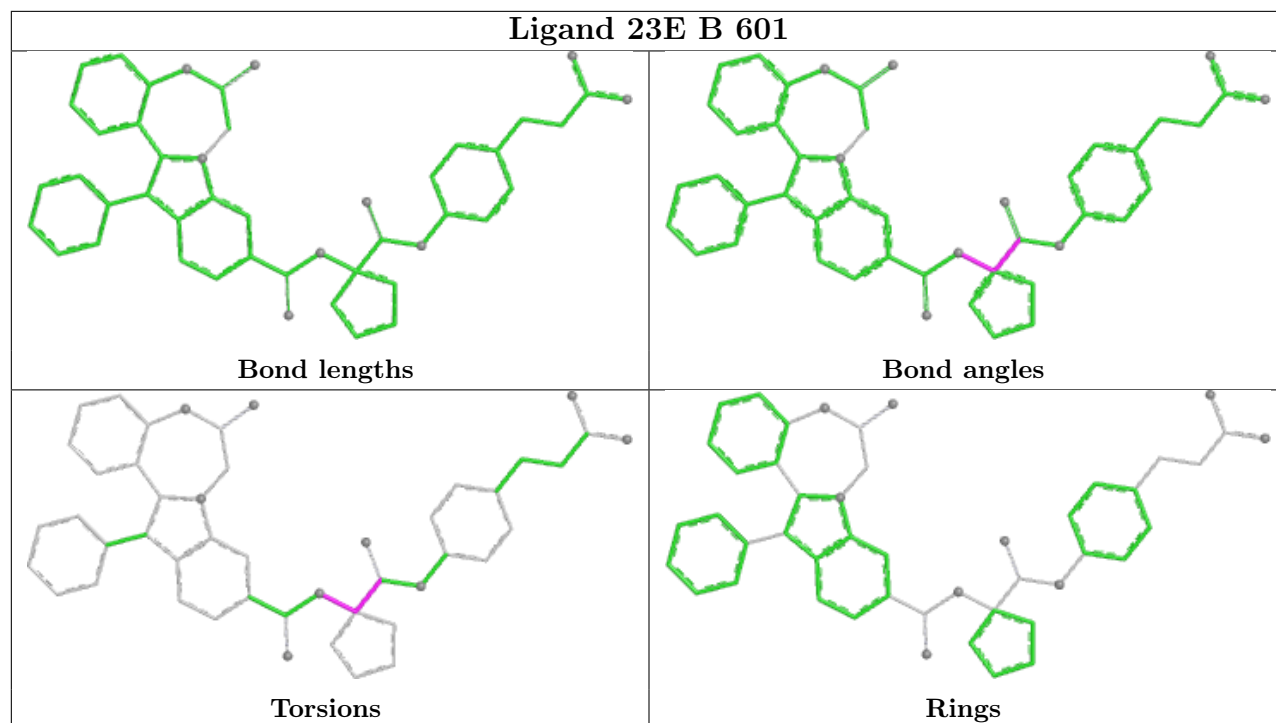
There are no ring outliers.

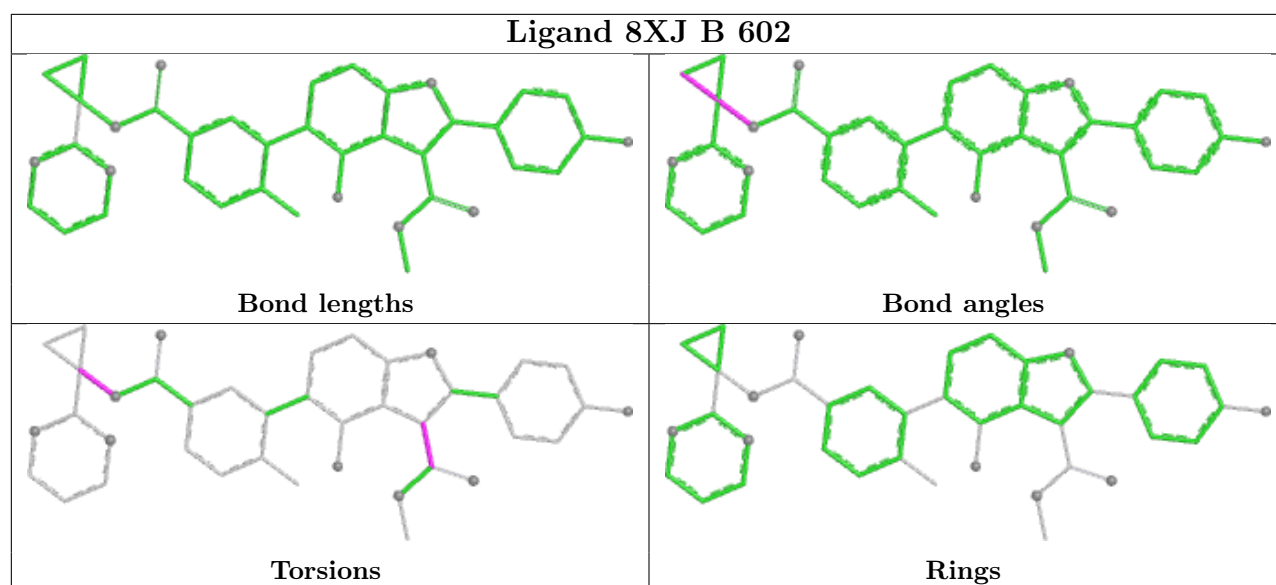
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	609	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	545/574 (94%)	0.04	21 (3%)	43 35	27, 56, 112, 152	0
1	B	535/574 (93%)	0.36	39 (7%)	21 18	37, 64, 145, 168	0
All	All	1080/1148 (94%)	0.20	60 (5%)	30 25	27, 60, 137, 168	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	553	ALA	5.3
1	A	554	GLY	4.4
1	B	550	TRP	4.3
1	B	552	VAL	4.3
1	A	147	VAL	4.1
1	B	147	VAL	4.0
1	B	554	GLY	3.9
1	B	12	THR	3.8
1	B	39	ALA	3.8
1	B	144	VAL	3.7
1	B	561	TYR	3.7
1	B	10	LEU	3.7
1	B	41	THR	3.7
1	A	555	TYR	3.6
1	B	148	GLN	3.4
1	B	547	LEU	3.4
1	B	558	GLY	3.4
1	B	562	HIS	3.2
1	B	149	PRO	3.1
1	B	159	LEU	3.1
1	A	144	VAL	3.0
1	B	555	TYR	3.0
1	B	13	PRO	3.0
1	B	549	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	551	PHE	3.0
1	A	567	ALA	2.9
1	A	552	VAL	2.9
1	A	13	PRO	2.8
1	B	38	TYR	2.8
1	B	47	LEU	2.8
1	B	557	GLY	2.8
1	A	39	ALA	2.7
1	B	545	LEU	2.7
1	B	138	ILE	2.7
1	B	160	ILE	2.6
1	A	40	THR	2.6
1	B	11	ILE	2.5
1	A	148	GLN	2.5
1	A	12	THR	2.4
1	B	146	CYS	2.4
1	B	559	ASP	2.4
1	A	532	THR	2.4
1	B	560	ILE	2.4
1	A	45	ALA	2.3
1	A	149	PRO	2.3
1	B	213	CYS	2.3
1	B	451	CYS	2.3
1	B	156	PRO	2.3
1	A	105	ALA	2.3
1	B	45	ALA	2.3
1	B	556	SER	2.3
1	A	569	PRO	2.2
1	A	10	LEU	2.2
1	A	568	ARG	2.2
1	A	42	SER	2.2
1	B	402	HIS	2.2
1	A	38	TYR	2.1
1	B	161	VAL	2.1
1	B	535	LYS	2.1
1	A	157	ALA	2.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

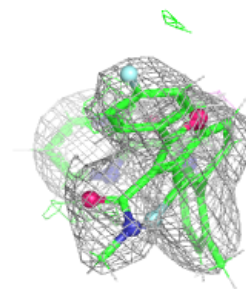
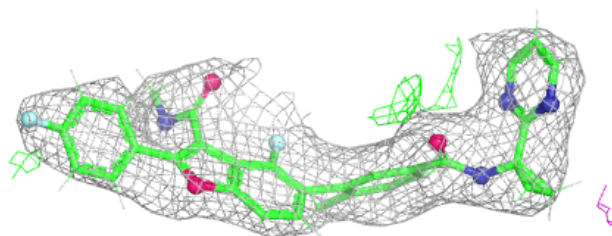
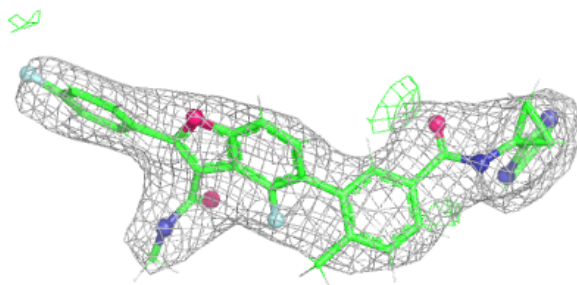
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	609	6/6	0.67	0.18	87,90,93,95	0
4	SO4	B	605	5/5	0.68	0.16	112,112,113,114	0
4	SO4	A	606	5/5	0.75	0.18	126,129,129,130	0
5	GOL	B	607	6/6	0.78	0.19	65,68,70,71	0
4	SO4	A	605	5/5	0.79	0.20	117,121,121,122	0
4	SO4	B	606	5/5	0.79	0.11	117,119,120,120	0
5	GOL	A	607	6/6	0.86	0.14	68,69,74,76	0
4	SO4	B	603	5/5	0.87	0.08	119,120,121,122	0
5	GOL	A	608	6/6	0.87	0.16	55,64,70,70	0
4	SO4	A	604	5/5	0.88	0.16	92,95,96,97	0
4	SO4	B	604	5/5	0.90	0.13	83,84,87,87	0
3	8XJ	B	602	40/40	0.95	0.08	43,49,54,59	24
2	23E	A	601	47/47	0.95	0.08	32,42,56,72	38
2	23E	B	601	47/47	0.95	0.09	45,49,70,80	38
3	8XJ	A	602	40/40	0.96	0.08	33,46,57,58	24
4	SO4	A	603	5/5	0.97	0.06	63,64,65,67	0

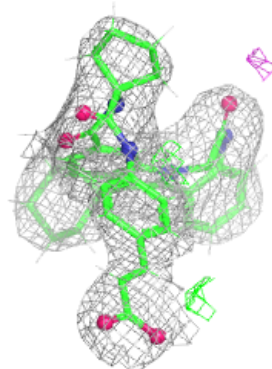
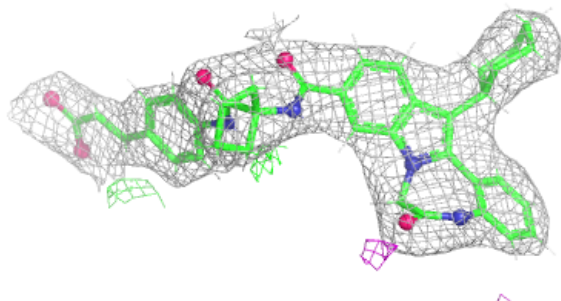
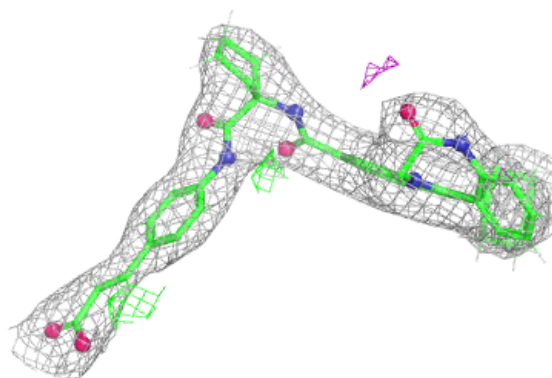
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8XJ 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)

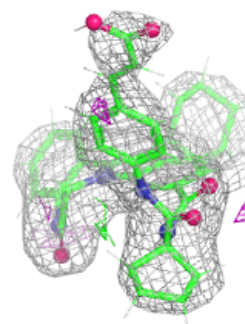
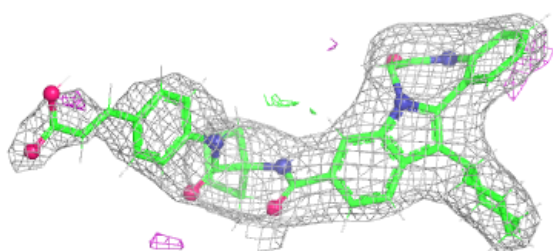
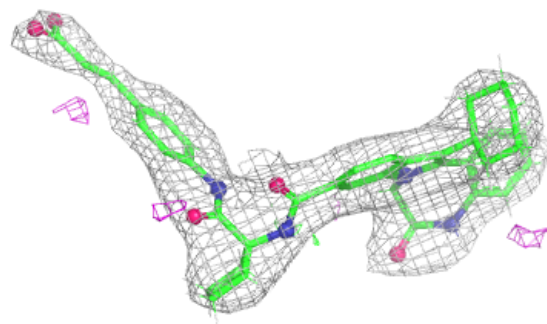
**Electron density around 23E A 601:**

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

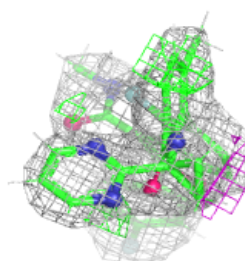
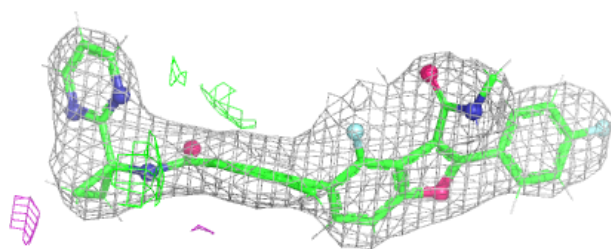
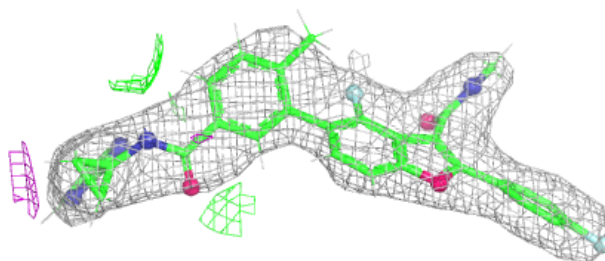


Electron density around 23E B 601:

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

**Electron density around 8XJ 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.