



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:46 AM UTC

PDB ID : 6NPV / pdb_00006npv
Title : C-abl Kinase domain with the activator(cmpd51), N-(1-(3,4-dichlorophenyl)-4-(2-hydroxyethyl)-4,5-dihydro-1H-pyrazol-3-yl)isonicotinamide
Authors : campobasso, N.
Deposited on : 2019-01-18
Resolution : 1.86 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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

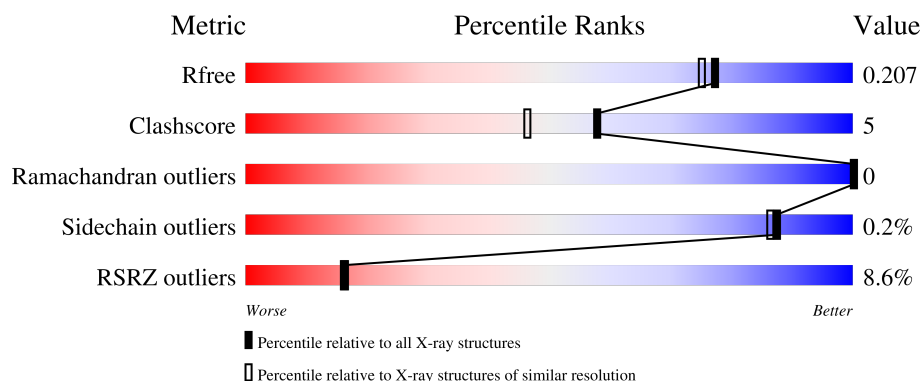
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	298	
1	B	298	

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
5	GOL	B	604	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4670 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 Tyrosine-protein kinase ABL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2129	1377	345	391	16			
1	B	257	Total	C	N	O	S	0	1	0
			2101	1358	339	388	16			

There are 28 discrepancies between the modelled and reference sequences:

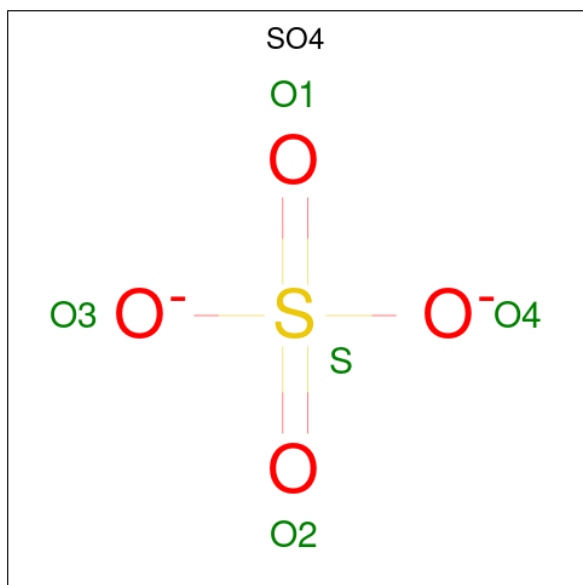
Chain	Residue	Modelled	Actual	Comment	Reference
A	234	MET	-	expression tag	UNP P00519
A	235	HIS	-	expression tag	UNP P00519
A	236	HIS	-	expression tag	UNP P00519
A	237	HIS	-	expression tag	UNP P00519
A	238	HIS	-	expression tag	UNP P00519
A	239	HIS	-	expression tag	UNP P00519
A	240	HIS	-	expression tag	UNP P00519
A	241	GLU	-	expression tag	UNP P00519
A	242	ASN	-	expression tag	UNP P00519
A	243	LEU	-	expression tag	UNP P00519
A	244	TYR	-	expression tag	UNP P00519
A	245	PHE	-	expression tag	UNP P00519
A	246	GLN	-	expression tag	UNP P00519
A	247	GLY	-	expression tag	UNP P00519
B	234	MET	-	expression tag	UNP P00519
B	235	HIS	-	expression tag	UNP P00519
B	236	HIS	-	expression tag	UNP P00519
B	237	HIS	-	expression tag	UNP P00519
B	238	HIS	-	expression tag	UNP P00519
B	239	HIS	-	expression tag	UNP P00519
B	240	HIS	-	expression tag	UNP P00519
B	241	GLU	-	expression tag	UNP P00519
B	242	ASN	-	expression tag	UNP P00519
B	243	LEU	-	expression tag	UNP P00519
B	244	TYR	-	expression tag	UNP P00519

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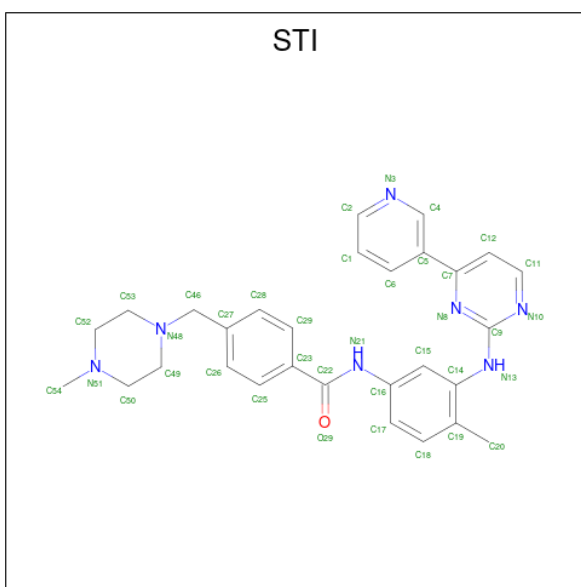
Chain	Residue	Modelled	Actual	Comment	Reference
B	245	PHE	-	expression tag	UNP P00519
B	246	GLN	-	expression tag	UNP P00519
B	247	GLY	-	expression tag	UNP P00519

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



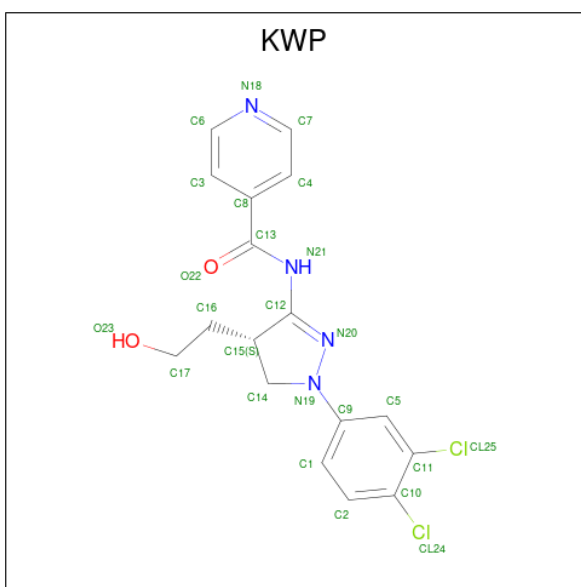
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 4-(4-METHYL-PIPERAZIN-1-YLMETHYL)-N-[4-METHYL-3-(4-PYRIDIN-3-YL-PYRIMIDIN-2-YLAMINO)-PHENYL]-BENZAMIDE (CCD ID: STI) (formula: C₂₉H₃₁N₇O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			37	29	7	1		
3	B	1	Total	C	N	O	0	0
			37	29	7	1		

- Molecule 4 is {N}-[(4 {S})-2-(3,4-dichlorophenyl)-4-(2-hydroxyethyl)-3,4-dihydropyrazol-5-yl]pyridine-4-carboxamide (CCD ID: KWP) (formula: C₁₇H₁₆Cl₂N₄O₂) (labeled as "Ligand of Interest" by depositor).



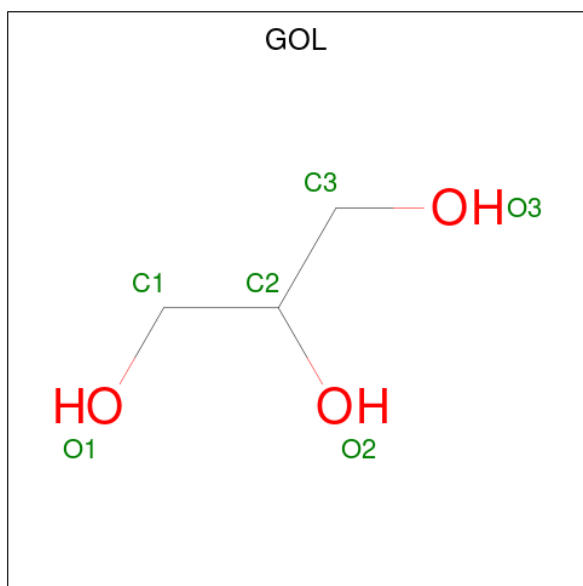
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0
			25	17	2	4	2	

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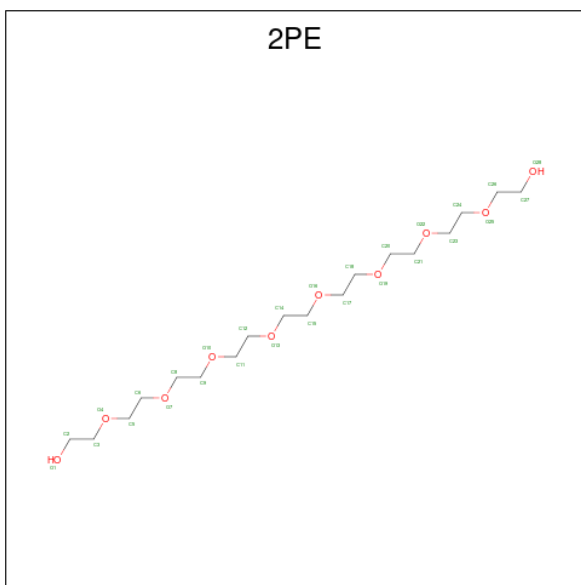
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	0	0
			25	17	2	4	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			28	18	10		

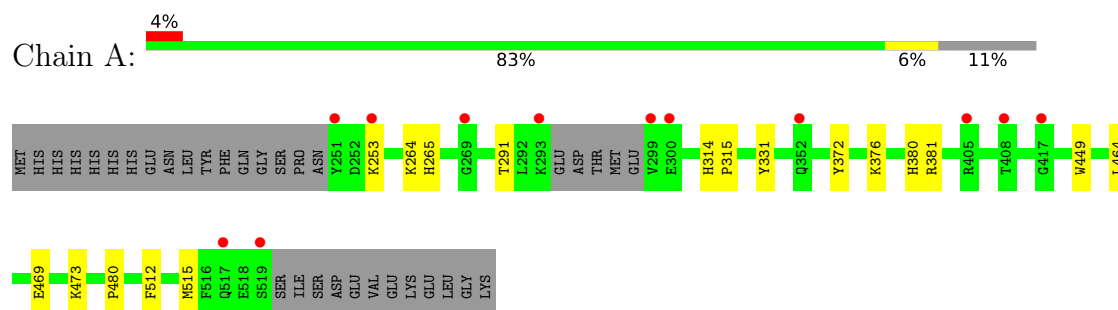
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	141	Total O 141 141	0	0
7	B	120	Total O 120 120	0	0

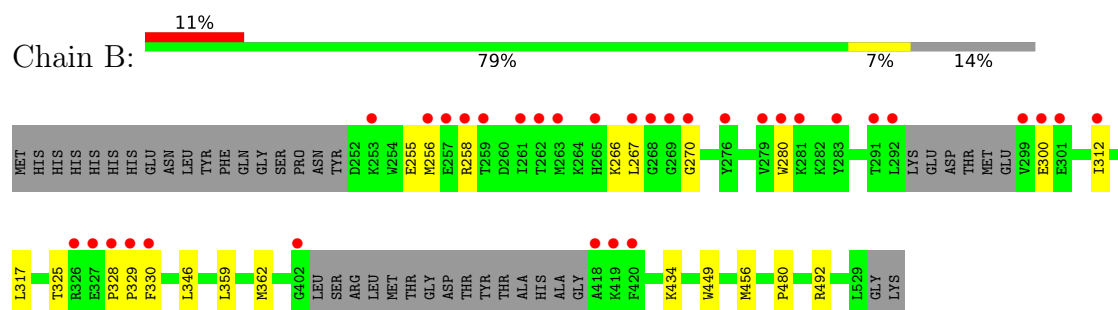
3 Residue-property plots [i](#)

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: Tyrosine-protein kinase ABL1



- Molecule 1: Tyrosine-protein kinase ABL1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.97Å 95.29Å 115.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.72 – 1.86 45.72 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.72-1.86) 99.8 (45.72-1.86)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 1.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.182 , 0.207 0.184 , 0.207	Depositor DCC
R_{free} test set	3497 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4670	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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: SO4, STI, KWP, 2PE, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/2184	0.49	0/2957
1	B	0.29	0/2156	0.47	0/2915
All	All	0.31	0/4340	0.48	0/5872

There are no bond length outliers.

There are no bond angle outliers.

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	2129	0	2071	12	0
1	B	2101	0	2057	24	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
3	A	37	0	31	1	0
3	B	37	0	31	1	0
4	A	25	0	0	0	0
4	B	25	0	0	0	0
5	B	12	0	16	5	0
6	B	28	0	38	8	0
7	A	141	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	120	0	0	1	0
All	All	4670	0	4244	39	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 5.

All (39) 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:434:LYS:HD2	6:B:606:2PE:H82	1.52	0.92
1:B:434:LYS:HZ3	6:B:606:2PE:H61	1.42	0.82
1:B:258:ARG:NH2	1:B:329:PRO:O	2.16	0.78
1:B:434:LYS:HZ1	6:B:606:2PE:H172	1.54	0.71
1:B:492:ARG:HE	5:B:604:GOL:H2	1.57	0.68
1:B:492:ARG:HH11	5:B:604:GOL:H2	1.62	0.65
1:B:346:LEU:HD21	1:B:362:MET:HE1	1.81	0.61
1:B:434:LYS:NZ	6:B:606:2PE:H61	2.16	0.61
1:B:434:LYS:NZ	6:B:606:2PE:H172	2.18	0.56
1:B:255:GLU:OE2	1:B:325:THR:OG1	2.21	0.56
1:A:253:LYS:HD3	1:A:253:LYS:N	2.24	0.53
1:B:434:LYS:HZ2	6:B:606:2PE:H141	1.74	0.52
1:B:492:ARG:NE	5:B:604:GOL:H2	2.25	0.51
1:B:300:GLU:N	1:B:300:GLU:OE2	2.41	0.50
1:B:456[B]:MET:HE3	7:B:746:HOH:O	2.12	0.49
1:A:264:LYS:NZ	7:A:703:HOH:O	2.46	0.48
1:A:291:THR:HG22	1:A:331:TYR:CD1	2.49	0.47
1:A:265:HIS:CD2	1:A:265:HIS:H	2.31	0.47
1:B:449:TRP:CD1	1:B:480:PRO:HG3	2.50	0.46
1:B:267:LEU:HD12	1:B:267:LEU:HA	1.81	0.46
3:A:602:STI:O29	3:A:602:STI:H151	2.15	0.46
1:A:372:TYR:OH	1:A:376:LYS:HE2	2.17	0.45
1:A:512:PHE:HA	1:A:515:MET:HE3	1.99	0.45
1:B:328:PRO:HG3	1:B:330:PHE:CZ	2.51	0.45
1:B:492:ARG:NH1	5:B:604:GOL:H2	2.28	0.45
1:A:380:HIS:O	1:A:381:ARG:HB2	2.17	0.44
1:B:492:ARG:HH11	5:B:604:GOL:C2	2.30	0.44
1:A:469:GLU:HG2	1:A:473:LYS:HE2	2.01	0.43
1:B:256:MET:HE1	1:B:280:TRP:CE2	2.53	0.43
1:B:312:ILE:HG23	1:B:317:LEU:HD13	2.01	0.43
6:B:606:2PE:H121	6:B:606:2PE:H271	2.01	0.42
1:A:449:TRP:CD1	1:A:480:PRO:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LYS:CD	1:A:253:LYS:H	2.33	0.42
1:B:266:LYS:HD3	1:B:270:GLY:HA2	2.02	0.41
3:B:603:STI:H151	3:B:603:STI:O29	2.20	0.41
1:A:314:HIS:CG	1:A:315:PRO:HD2	2.56	0.41
1:A:253:LYS:N	1:A:253:LYS:CD	2.84	0.41
1:B:434:LYS:NZ	6:B:606:2PE:H141	2.35	0.41
1:B:359:LEU:HA	1:B:362:MET:HE2	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	260/298 (87%)	253 (97%)	7 (3%)	0	100	100
1	B	252/298 (85%)	245 (97%)	7 (3%)	0	100	100
All	All	512/596 (86%)	498 (97%)	14 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	224/262 (86%)	223 (100%)	1 (0%)	84	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	226/262 (86%)	226 (100%)	0	100	100
All	All	450/524 (86%)	449 (100%)	1 (0%)	87	86

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	464	LEU

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

Mol	Chain	Res	Type
1	A	352	GLN
1	A	510	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 ⓘ

10 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	SO4	B	601	-	4,4,4	0.19	0	6,6,6	0.24	0
4	KWP	A	603	-	25,27,27	1.15	3 (12%)	29,37,37	1.42	4 (13%)
5	GOL	B	604	-	5,5,5	0.35	0	5,5,5	0.99	0
2	SO4	A	601	-	4,4,4	0.24	0	6,6,6	0.09	0
6	2PE	B	606	-	27,27,27	0.55	0	26,26,26	0.95	0
5	GOL	B	605	-	5,5,5	0.45	0	5,5,5	0.31	0
3	STI	B	603	-	41,41,41	0.14	0	56,56,56	0.34	0
4	KWP	B	607	-	25,27,27	1.16	3 (12%)	29,37,37	1.38	3 (10%)
2	SO4	B	602	-	4,4,4	0.25	0	6,6,6	0.10	0
3	STI	A	602	-	41,41,41	0.18	0	56,56,56	0.32	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
5	GOL	B	604	-	-	4/4/4/4	-
4	KWP	A	603	-	-	0/14/27/27	0/3/3/3
6	2PE	B	606	-	-	16/25/25/25	-
5	GOL	B	605	-	-	0/4/4/4	-
3	STI	B	603	-	-	2/20/30/30	0/5/5/5
4	KWP	B	607	-	-	3/14/27/27	0/3/3/3
3	STI	A	602	-	-	2/20/30/30	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	KWP	N19-N20	3.60	1.43	1.36
4	B	607	KWP	N19-N20	3.52	1.43	1.36
4	B	607	KWP	C12-N21	-2.86	1.33	1.36
4	B	607	KWP	C13-N21	2.79	1.42	1.37
4	A	603	KWP	C13-N21	2.53	1.42	1.37
4	A	603	KWP	C12-N21	-2.41	1.33	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	607	KWP	C5-C9-N19	-4.11	117.27	120.30
4	A	603	KWP	C5-C9-N19	-4.08	117.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	KWP	C14-C15-C12	2.95	105.96	101.67
4	A	603	KWP	C1-C9-N19	2.45	123.32	120.31
4	B	607	KWP	C1-C9-N19	2.30	123.14	120.31
4	B	607	KWP	C14-C15-C12	2.27	104.97	101.67
4	A	603	KWP	C6-C3-C8	-2.02	116.84	119.05

There are no chirality outliers.

All (27) torsion outliers are listed below:

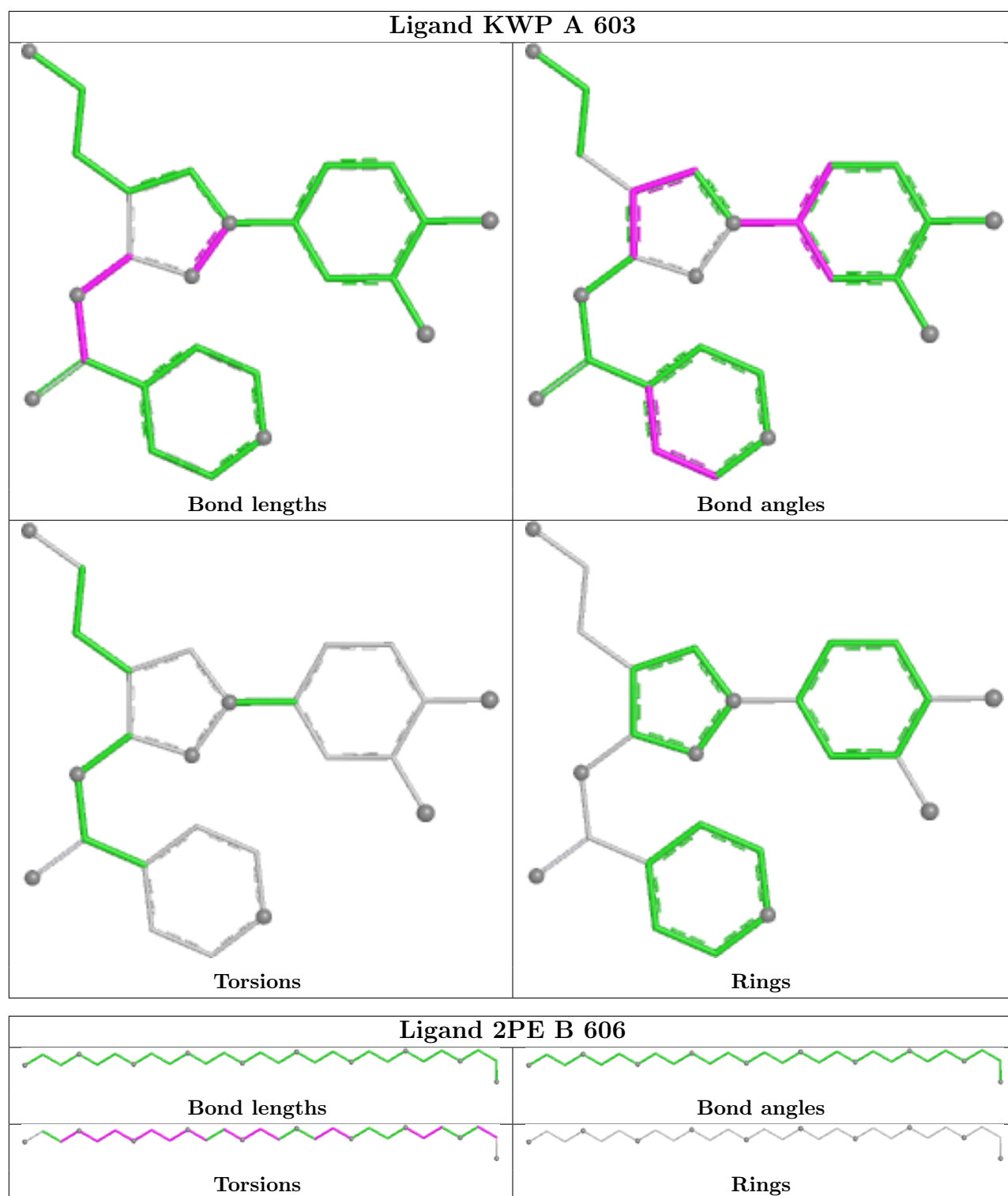
Mol	Chain	Res	Type	Atoms
3	A	602	STI	C19-C14-N13-C9
3	A	602	STI	C15-C14-N13-C9
3	B	603	STI	C19-C14-N13-C9
3	B	603	STI	C15-C14-N13-C9
4	B	607	KWP	C12-C15-C16-C17
4	B	607	KWP	C14-C15-C16-C17
5	B	604	GOL	O1-C1-C2-C3
5	B	604	GOL	C1-C2-C3-O3
6	B	606	2PE	C27-C26-O25-C24
6	B	606	2PE	C21-C20-O19-C18
6	B	606	2PE	O4-C5-C6-O7
6	B	606	2PE	O10-C11-C12-O13
6	B	606	2PE	O19-C20-C21-O22
5	B	604	GOL	O2-C2-C3-O3
6	B	606	2PE	C20-C21-O22-C23
6	B	606	2PE	C14-C15-O16-C17
5	B	604	GOL	O1-C1-C2-O2
6	B	606	2PE	O1-C2-C3-O4
6	B	606	2PE	C18-C17-O16-C15
6	B	606	2PE	C17-C18-O19-C20
6	B	606	2PE	C24-C23-O22-C21
4	B	607	KWP	C15-C16-C17-O23
6	B	606	2PE	C5-C6-O7-C8
6	B	606	2PE	C23-C24-O25-C26
6	B	606	2PE	C12-C11-O10-C9
6	B	606	2PE	O22-C23-C24-O25
6	B	606	2PE	O13-C14-C15-O16

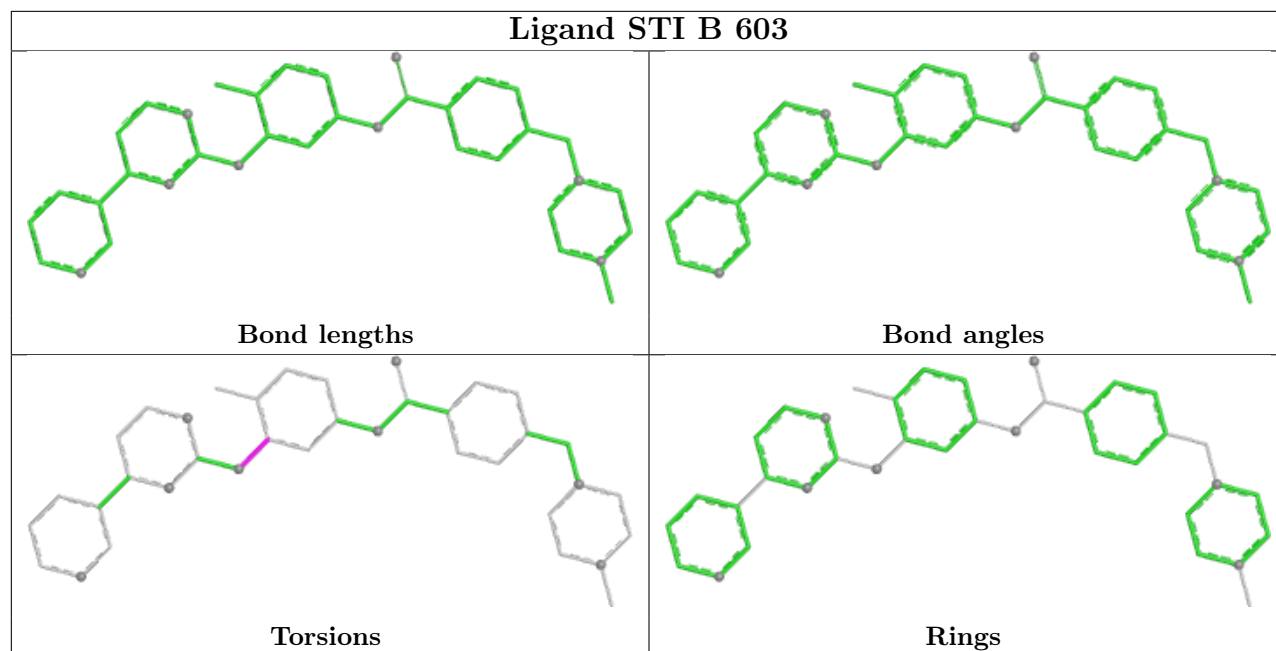
There are no ring outliers.

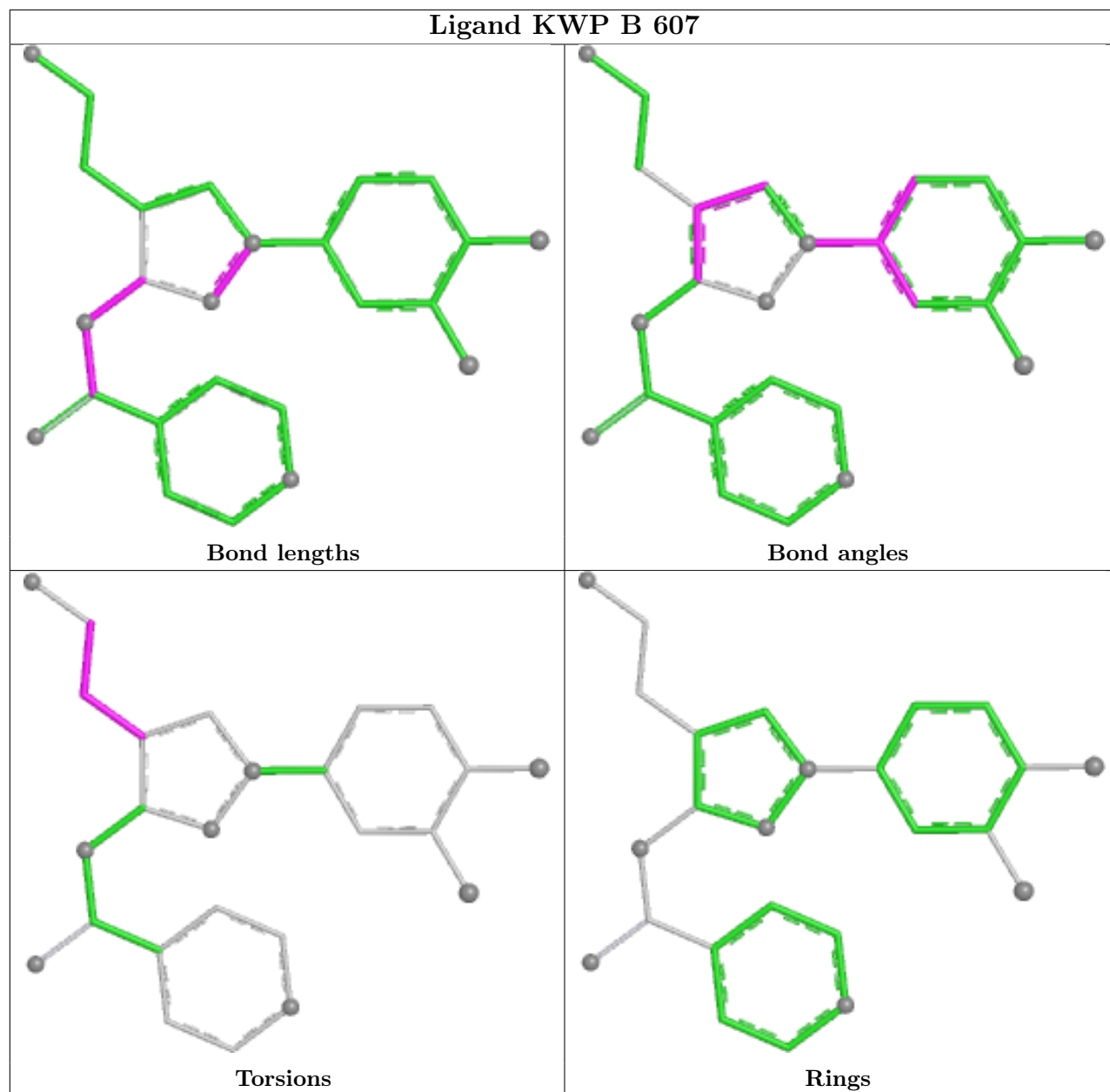
4 monomers are involved in 15 short contacts:

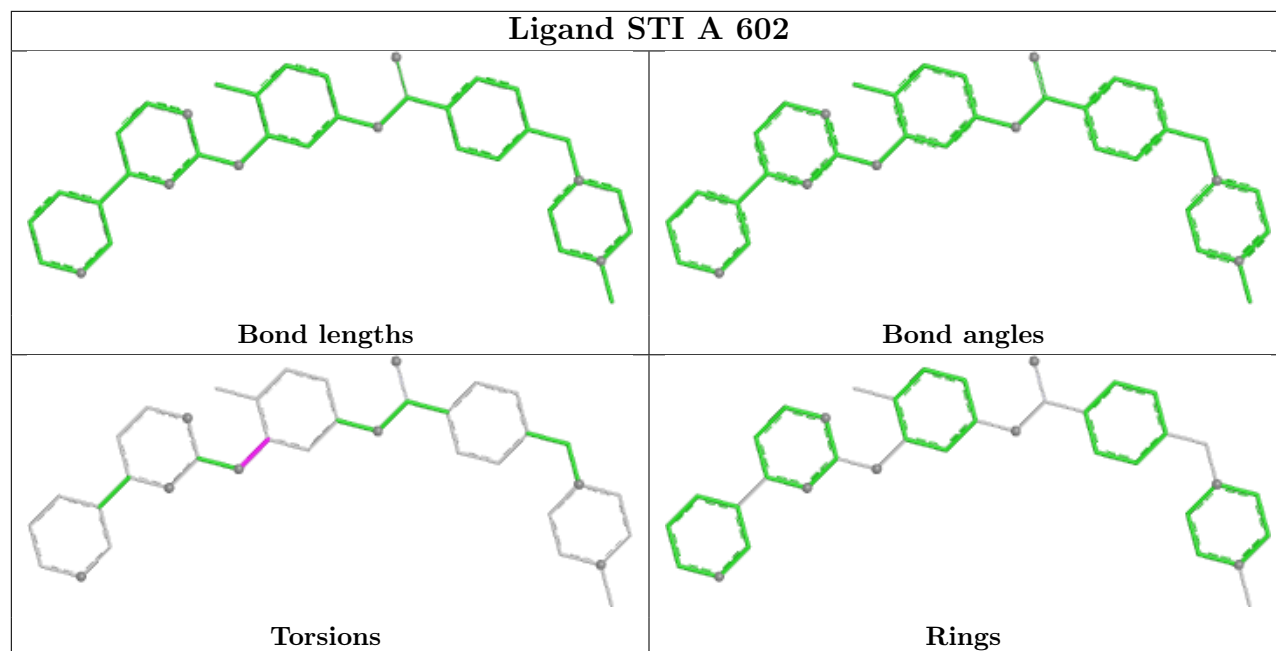
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	604	GOL	5	0
6	B	606	2PE	8	0
3	B	603	STI	1	0
3	A	602	STI	1	0

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	264/298 (88%)	0.12	12 (4%) 38 41	13, 23, 45, 57	0
1	B	257/298 (86%)	0.39	33 (12%) 7 7	13, 24, 58, 75	1 (0%)
All	All	521/596 (87%)	0.25	45 (8%) 16 16	13, 23, 51, 75	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	299	VAL	9.6
1	B	418	ALA	9.1
1	B	420	PHE	6.0
1	A	299	VAL	5.3
1	A	251	TYR	4.5
1	B	292	LEU	4.2
1	B	269	GLY	4.2
1	B	402	GLY	4.1
1	A	405	ARG	3.9
1	B	330	PHE	3.7
1	A	408	THR	3.6
1	B	265	HIS	3.6
1	B	419	LYS	3.6
1	B	328	PRO	3.5
1	B	257	GLU	3.3
1	B	300	GLU	3.3
1	B	258	ARG	3.2
1	B	327	GLU	3.1
1	B	329	PRO	3.1
1	B	280	TRP	3.1
1	B	261	ILE	3.0
1	B	283	TYR	2.9
1	B	291	THR	2.9
1	A	293	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	269	GLY	2.7
1	A	519	SER	2.7
1	A	253	LYS	2.7
1	B	256	MET	2.6
1	B	276	TYR	2.5
1	B	259	THR	2.5
1	B	267	LEU	2.4
1	B	301	GLU	2.4
1	B	326	ARG	2.4
1	B	312	ILE	2.3
1	B	262	THR	2.3
1	A	517	GLN	2.2
1	B	263	MET	2.2
1	B	270	GLY	2.2
1	A	352	GLN	2.1
1	A	417	GLY	2.1
1	B	268	GLY	2.1
1	B	279	VAL	2.1
1	A	300	GLU	2.0
1	B	253	LYS	2.0
1	B	281	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 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($\text{\AA}^2$)	Q<0.9
2	SO4	B	602	5/5	0.56	0.16	48,66,75,79	0
6	2PE	B	606	28/28	0.80	0.19	40,49,55,61	0

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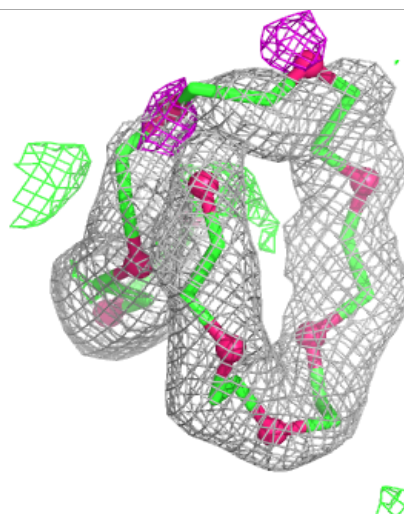
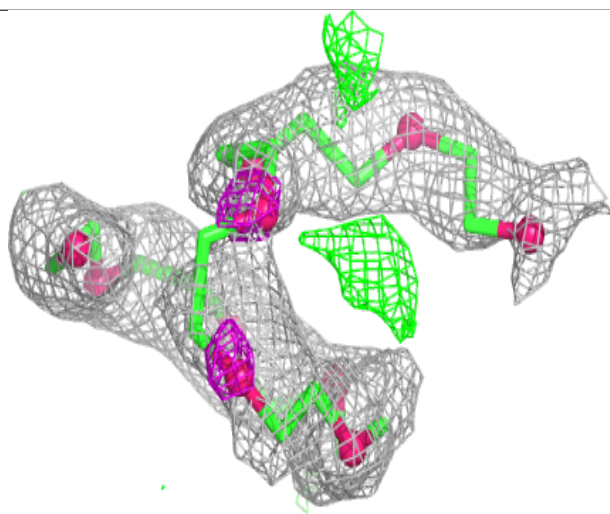
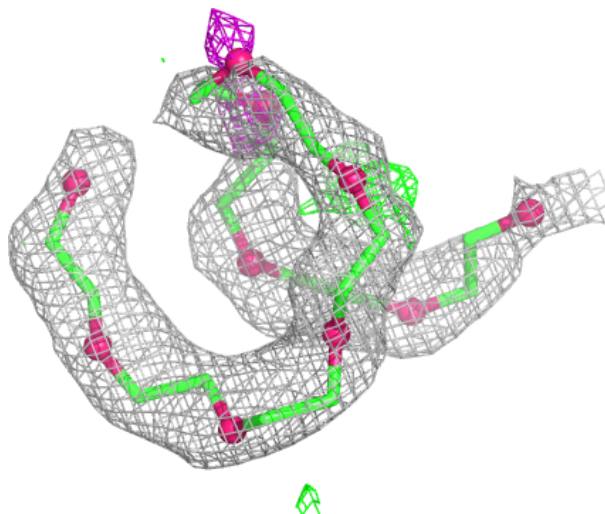
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	B	605	6/6	0.82	0.18	24,33,35,36	0
2	SO4	A	601	5/5	0.89	0.10	49,50,55,56	0
5	GOL	B	604	6/6	0.93	0.13	17,32,37,37	0
2	SO4	B	601	5/5	0.94	0.11	33,38,41,45	0
4	KWP	B	607	25/25	0.96	0.08	15,21,28,36	0
3	STI	B	603	37/37	0.96	0.07	23,28,31,32	0
3	STI	A	602	37/37	0.97	0.06	15,19,27,29	0
4	KWP	A	603	25/25	0.97	0.07	17,22,28,37	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.

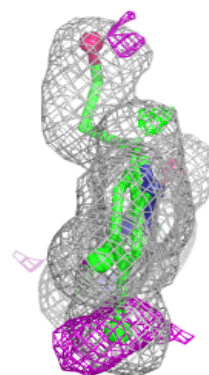
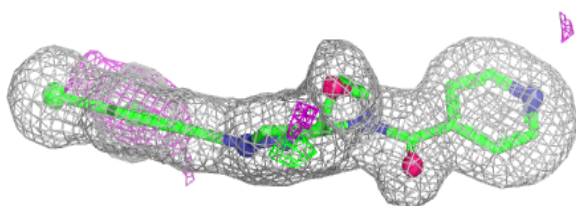
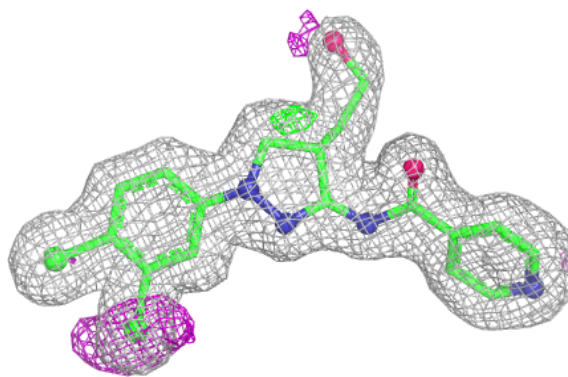
Electron density around 2PE B 606:

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

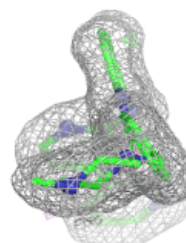
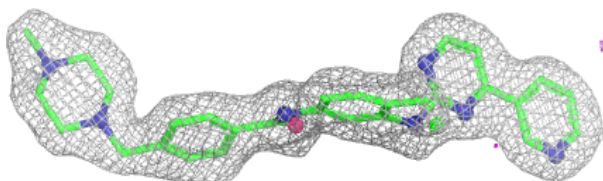
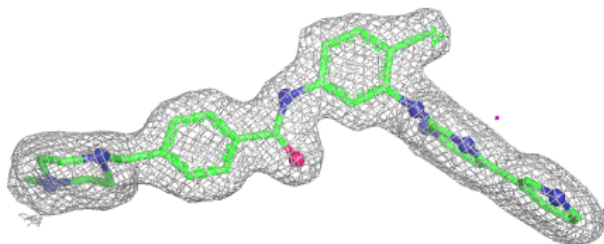


Electron density around KWP B 607:

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

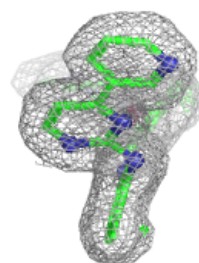
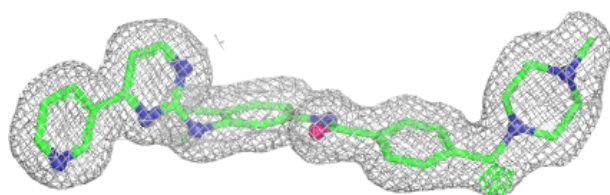
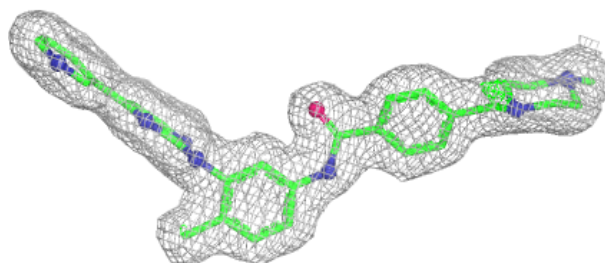
**Electron density around STI B 603:**

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

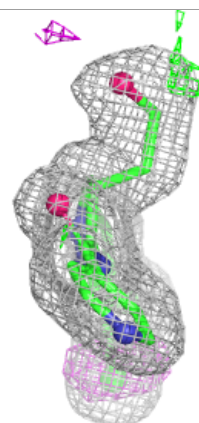
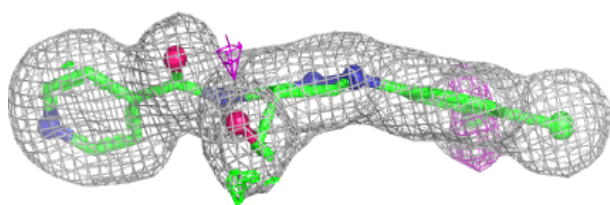
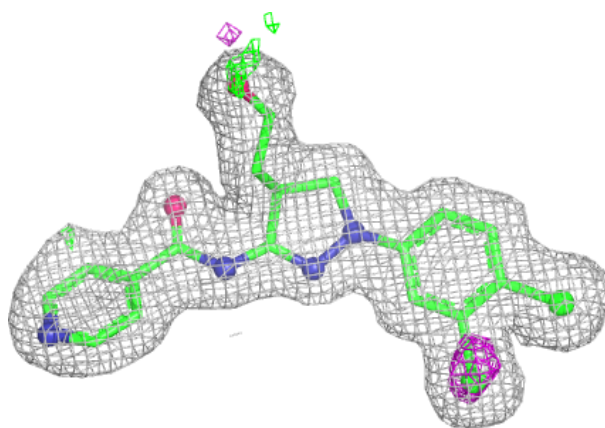


Electron density around STI A 602:

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

**Electron density around KWP A 603:**

$2mF_o-DF_c$ (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.