Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2024 – 08:12 PM EST

PDB ID	:	6NPU
Title	:	C-abl Kinase domain with the activator(cmpd29), N-(1-(3,4-dichlorophenyl)-4,5-dihydro-1H-pyrazol-3-yl)acetamide
Authors	:	Campobasso, N.
Deposited on	:	2019-01-18
Resolution	:	2.33 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 (i) 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 (i)) were used in the production of this report:

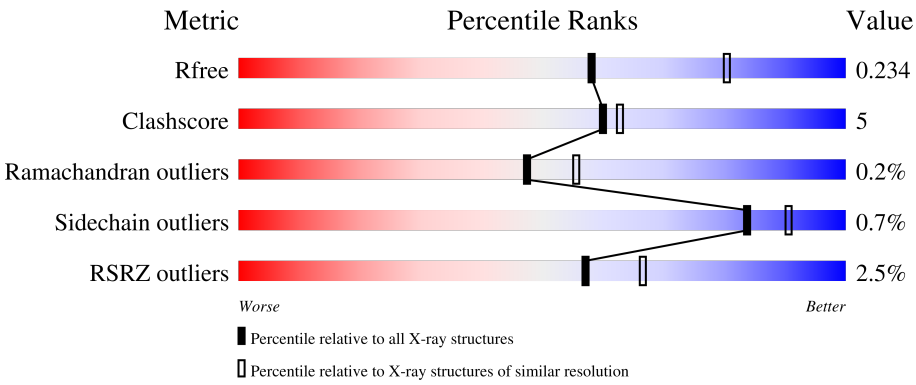
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 <=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	2% 81% 7% 11%
1	B	298	2% 78% 8% 14%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4456 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
			Total	C	N	O	S			
1	A	264	2135	1380	348	391	16	0	0	0
1	B	257	2096	1354	339	388	15	0	0	0

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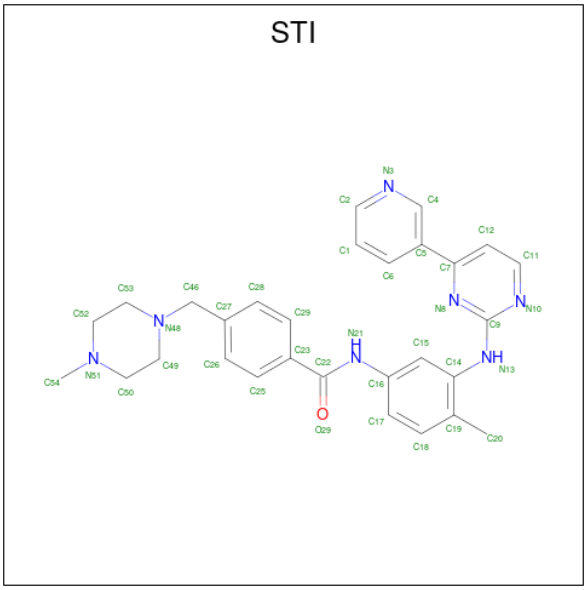
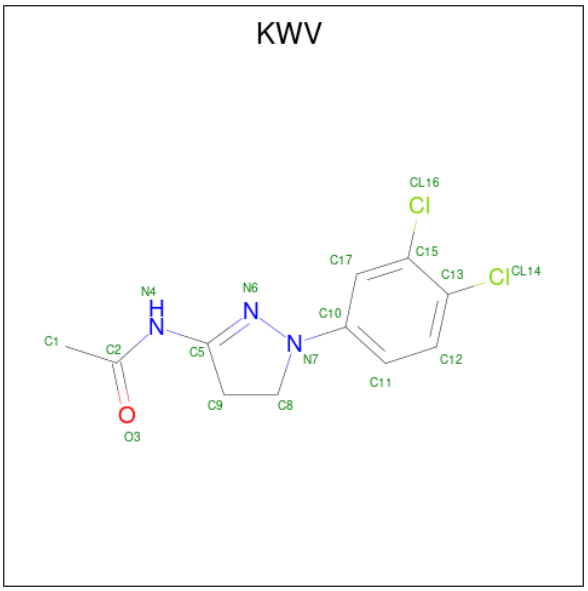
Chain	Residue	Modelled	Actual	Comment	Reference
B	245	PHE	-	expression tag	UNP P00519
B	246	GLN	-	expression tag	UNP P00519
B	247	GLY	-	expression tag	UNP P00519

- Molecule 2 is 4-(4-METHYL-PIPERAZIN-1-YLMETHYL)-N-[4-METHYL-3-(4-PYRIDIN-3-YL-PYRIMIDIN-2-YLAMINO)-PHENYL]-BENZAMIDE (three-letter code: STI) (formula: $C_{29}H_{31}N_7O$).



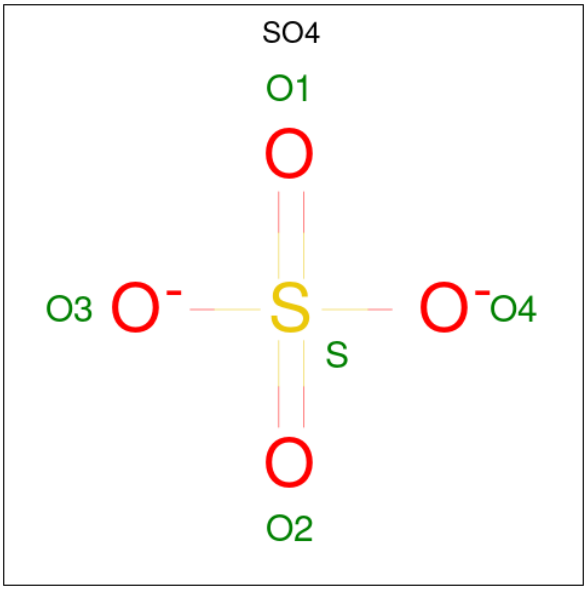
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	37	29	7	1	0	0
			Total	C	N	O		
2	B	1	37	29	7	1	0	0

- Molecule 3 is {N}-[2-(3,4-dichlorophenyl)-3,4-dihydropyrazol-5-yl]ethanamide (three-letter code: KWV) (formula: $C_{11}H_{11}Cl_2N_3O$).



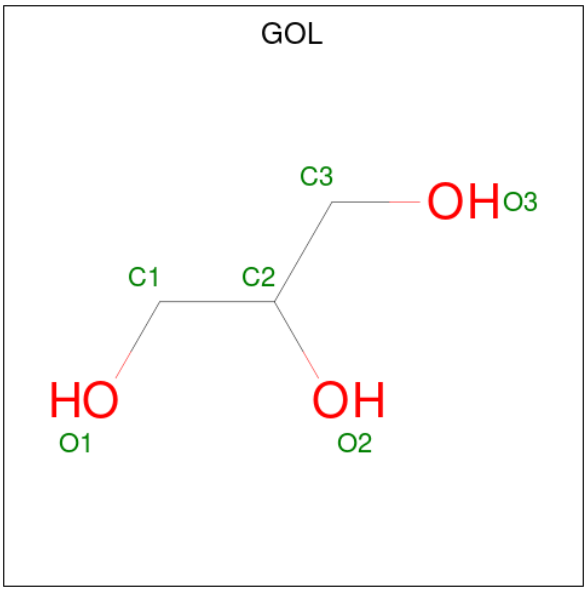
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			17	11	2	3	1		
3	B	1	Total	C	Cl	N	O	0	0
			17	11	2	3	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



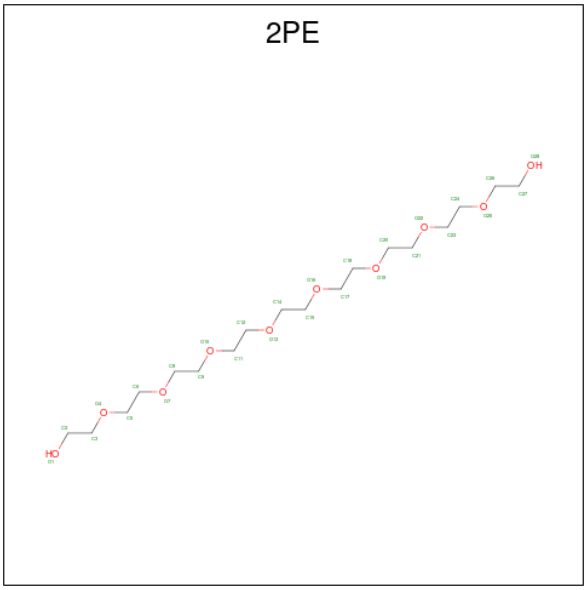
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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



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

- Molecule 7 is water.

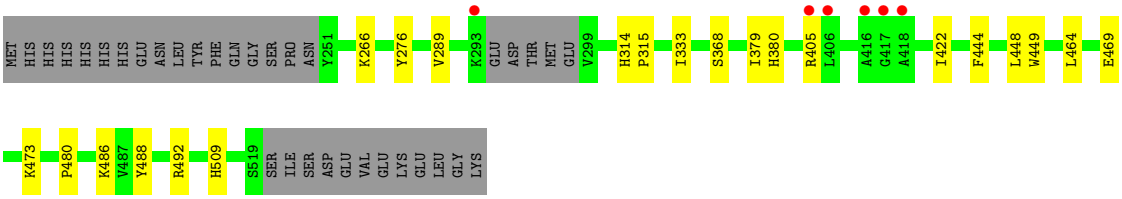
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	42	42	42	0	0
			Total	O		
7	B	30	30	30	0	0

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.

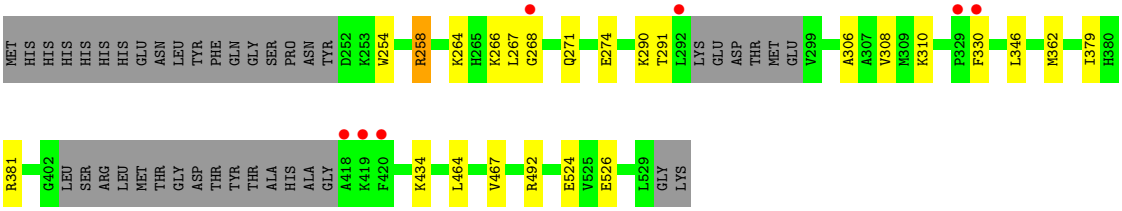
• Molecule 1: Tyrosine-protein kinase ABL1

Chain A:



• Molecule 1: Tyrosine-protein kinase ABL1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.09Å 95.64Å 115.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.70 – 2.33 73.67 – 2.33	Depositor EDS
% Data completeness (in resolution range)	95.9 (73.70-2.33) 89.8 (73.67-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.193 , 0.234 0.193 , 0.234	Depositor DCC
R_{free} test set	1780 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4456	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, STI, KWV, 2PE, 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	0.46	0/2190	0.57	0/2964
1	B	0.44	0/2148	0.57	0/2905
All	All	0.45	0/4338	0.57	0/5869

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	2135	0	2082	15	0
1	B	2096	0	2048	21	0
2	A	37	0	31	2	0
2	B	37	0	31	2	0
3	A	17	0	0	0	0
3	B	17	0	0	3	0
4	B	5	0	0	0	0
5	B	12	0	16	2	0
6	B	28	0	38	7	0
7	A	42	0	0	0	0
7	B	30	0	0	1	0
All	All	4456	0	4246	40	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 (40) 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)
3:B:605:KWV:N6	3:B:605:KWV:N7	1.60	1.10
1:B:434:LYS:HZ1	6:B:606:2PE:H172	1.34	0.93
1:A:289:VAL:HG13	1:A:333:ILE:HD13	1.67	0.77
1:B:526:GLU:OE2	7:B:701:HOH:O	2.07	0.72
1:B:434:LYS:HZ3	6:B:606:2PE:H61	1.53	0.71
1:B:258:ARG:HD3	1:B:258:ARG:H	1.58	0.68
1:B:434:LYS:NZ	6:B:606:2PE:H172	2.11	0.65
1:B:434:LYS:HD2	6:B:606:2PE:H82	1.78	0.65
1:A:379:ILE:O	2:A:601:STI:H501	1.96	0.65
1:A:289:VAL:HG13	1:A:333:ILE:CD1	2.28	0.64
1:B:290:LYS:HB2	2:B:602:STI:H181	1.81	0.61
1:B:346:LEU:HD21	1:B:362:MET:HE1	1.83	0.61
1:B:492:ARG:HH11	5:B:603:GOL:H2	1.65	0.61
1:B:434:LYS:NZ	6:B:606:2PE:H61	2.19	0.57
3:B:605:KWV:N6	3:B:605:KWV:C10	2.60	0.57
1:A:289:VAL:HG22	1:A:333:ILE:CD1	2.38	0.53
1:A:422:ILE:HB	1:A:464:LEU:HD22	1.91	0.52
1:B:492:ARG:NH1	5:B:603:GOL:H2	2.25	0.51
1:B:268:GLY:O	1:B:271:GLN:HG2	2.11	0.51
1:A:289:VAL:HG22	1:A:333:ILE:HD12	1.93	0.51
1:B:308:VAL:HG11	2:B:602:STI:H491	1.94	0.50
1:A:314:HIS:CG	1:A:315:PRO:HD2	2.47	0.50
1:A:469:GLU:HG2	1:A:473:LYS:HE2	1.94	0.50
1:A:449:TRP:CD1	1:A:480:PRO:HG3	2.46	0.49
1:B:266:LYS:NZ	1:B:274:GLU:OE2	2.47	0.47
1:A:266:LYS:HG3	1:A:276:TYR:CE2	2.49	0.47
1:B:379:ILE:HG22	1:B:381:ARG:HG3	1.97	0.47
1:A:368:SER:HB2	1:A:509:HIS:CD2	2.49	0.46
1:A:444:PHE:CZ	1:A:448:LEU:HD11	2.50	0.46
1:B:434:LYS:NZ	6:B:606:2PE:H141	2.30	0.46
1:A:380:HIS:O	2:A:601:STI:H521	2.16	0.45
1:A:488:TYR:CZ	1:A:492:ARG:HD3	2.51	0.45
1:B:464:LEU:HA	1:B:467:VAL:HG23	1.99	0.45
1:B:254:TRP:CD1	1:B:310:LYS:HD3	2.53	0.44
1:B:267:LEU:HD12	1:B:267:LEU:HA	1.72	0.44
3:B:605:KWV:N6	3:B:605:KWV:C17	2.80	0.44
6:B:606:2PE:H172	6:B:606:2PE:H141	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:THR:HA	1:B:330:PHE:O	2.19	0.42
1:B:306:ALA:O	1:B:310:LYS:HG3	2.18	0.42
1:A:486:LYS:HA	1:A:486:LYS:HD2	1.92	0.41

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%)	250 (96%)	10 (4%)	0	100	100
1	B	251/298 (84%)	241 (96%)	9 (4%)	1 (0%)	34	38
All	All	511/596 (86%)	491 (96%)	19 (4%)	1 (0%)	47	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	264	LYS

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	225/262 (86%)	224 (100%)	1 (0%)	91	95
1	B	225/262 (86%)	223 (99%)	2 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	450/524 (86%)	447 (99%)	3 (1%)	84 90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	ARG
1	B	258	ARG
1	B	524	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	KWV	B	605	-	17,18,18	4.46	7 (41%)	18,25,25	2.42	4 (22%)
4	SO4	B	601	-	4,4,4	0.15	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	B	603	-	5,5,5	0.70	0	5,5,5	1.21	1 (20%)
2	STI	A	601	-	40,41,41	3.00	21 (52%)	51,56,56	2.16	14 (27%)
6	2PE	B	606	-	27,27,27	0.53	0	26,26,26	0.68	0
5	GOL	B	604	-	5,5,5	1.52	2 (40%)	5,5,5	0.67	0
3	KWV	A	602	-	17,18,18	4.39	6 (35%)	18,25,25	2.26	4 (22%)
2	STI	B	602	-	40,41,41	3.09	20 (50%)	51,56,56	2.02	11 (21%)

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	KWV	B	605	-	-	0/7/17/17	0/2/2/2
5	GOL	B	603	-	-	4/4/4/4	-
2	STI	A	601	-	-	2/16/30/30	0/5/5/5
6	2PE	B	606	-	-	17/25/25/25	-
5	GOL	B	604	-	-	0/4/4/4	-
3	KWV	A	602	-	-	0/7/17/17	0/2/2/2
2	STI	B	602	-	-	1/16/30/30	0/5/5/5

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	605	KWV	N7-N6	11.92	1.60	1.36
3	A	602	KWV	N7-N6	11.64	1.60	1.36
2	B	602	STI	C46-N48	-10.15	1.27	1.47
2	A	601	STI	C46-N48	-9.73	1.28	1.47
3	A	602	KWV	C8-N7	-9.10	1.34	1.47
3	B	605	KWV	C8-N7	-9.02	1.34	1.47
2	B	602	STI	C54-N51	-8.56	1.26	1.46
3	A	602	KWV	C5-N4	7.98	1.49	1.37
2	A	601	STI	C54-N51	-7.93	1.28	1.46
3	B	605	KWV	C5-N4	7.89	1.49	1.37
2	B	602	STI	C9-N13	5.49	1.47	1.36
2	A	601	STI	C9-N13	5.35	1.47	1.36
3	B	605	KWV	C9-C5	4.17	1.57	1.50
3	B	605	KWV	C2-N4	4.05	1.44	1.37
3	A	602	KWV	C2-N4	3.92	1.44	1.37
2	B	602	STI	C9-N10	-3.90	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	STI	C22-N21	3.78	1.45	1.35
2	B	602	STI	C22-N21	3.74	1.45	1.35
2	A	601	STI	C50-N51	-3.64	1.38	1.46
3	A	602	KWV	C9-C5	3.61	1.56	1.50
2	B	602	STI	C50-N51	-3.40	1.39	1.46
2	B	602	STI	C52-N51	-3.39	1.39	1.46
2	A	601	STI	C53-N48	-3.37	1.37	1.46
2	A	601	STI	C28-C27	3.37	1.46	1.38
2	A	601	STI	C52-N51	-3.36	1.39	1.46
2	A	601	STI	C9-N10	-3.32	1.30	1.34
2	A	601	STI	C46-C27	3.31	1.57	1.51
2	B	602	STI	C53-N48	-3.27	1.37	1.46
2	B	602	STI	C12-C11	3.21	1.41	1.36
2	B	602	STI	C16-N21	3.20	1.48	1.41
2	A	601	STI	O29-C22	-3.17	1.16	1.23
2	A	601	STI	C12-C11	3.10	1.40	1.36
2	B	602	STI	C25-C23	3.05	1.44	1.39
2	B	602	STI	C46-C27	2.94	1.56	1.51
2	A	601	STI	C25-C23	2.91	1.44	1.39
2	A	601	STI	C16-N21	2.90	1.47	1.41
2	A	601	STI	C49-N48	-2.87	1.39	1.46
2	B	602	STI	C7-N8	-2.77	1.33	1.37
2	B	602	STI	C12-C7	-2.75	1.37	1.41
2	B	602	STI	O29-C22	-2.70	1.17	1.23
2	B	602	STI	C14-N13	2.70	1.47	1.39
2	A	601	STI	C7-N8	-2.68	1.33	1.37
3	B	605	KWV	C15-CL16	2.65	1.79	1.73
2	B	602	STI	C28-C27	2.64	1.44	1.38
2	B	602	STI	C23-C22	2.59	1.55	1.50
3	A	602	KWV	C15-CL16	2.58	1.79	1.73
2	B	602	STI	C49-N48	-2.56	1.39	1.46
2	A	601	STI	C14-N13	2.49	1.46	1.39
2	A	601	STI	C20-C19	2.48	1.56	1.51
2	A	601	STI	C12-C7	-2.32	1.37	1.41
3	B	605	KWV	O3-C2	-2.25	1.18	1.23
2	B	602	STI	C6-C5	-2.23	1.36	1.41
5	B	604	GOL	C1-C2	2.18	1.60	1.51
5	B	604	GOL	C3-C2	2.17	1.60	1.51
2	A	601	STI	C23-C22	2.07	1.54	1.50
2	A	601	STI	C6-C5	-2.06	1.37	1.41

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	KWV	C9-C8-N7	7.36	106.43	102.24
3	B	605	KWV	C17-C10-N7	-6.34	115.60	120.27
3	B	605	KWV	C9-C8-N7	6.28	105.82	102.24
2	B	602	STI	C11-N10-C9	5.70	120.50	115.45
2	A	601	STI	C49-C50-N51	5.62	117.16	110.80
2	A	601	STI	C11-N10-C9	5.42	120.26	115.45
2	B	602	STI	N10-C9-N8	-5.14	121.56	126.52
2	A	601	STI	C50-N51-C52	5.08	116.62	109.52
2	B	602	STI	C50-N51-C52	5.02	116.54	109.52
2	A	601	STI	C12-C11-N10	-4.78	119.10	123.81
2	B	602	STI	C12-C11-N10	-4.66	119.22	123.81
2	A	601	STI	C53-C52-N51	4.65	116.06	110.80
2	A	601	STI	N10-C9-N8	-4.62	122.06	126.52
2	B	602	STI	C49-C50-N51	4.32	115.68	110.80
3	A	602	KWV	C17-C10-N7	-4.04	117.29	120.27
2	B	602	STI	C9-N8-C7	4.00	122.11	115.60
2	A	601	STI	C9-N8-C7	3.53	121.36	115.60
2	B	602	STI	C14-N13-C9	-3.48	119.10	129.60
2	B	602	STI	C49-N48-C53	3.09	115.80	108.83
3	B	605	KWV	C1-C2-N4	2.98	120.44	115.29
2	A	601	STI	C49-N48-C53	2.82	115.17	108.83
2	B	602	STI	C18-C19-C14	2.68	119.96	117.44
2	A	601	STI	C28-C29-C23	-2.64	117.70	120.78
3	A	602	KWV	C1-C2-N4	2.61	119.80	115.29
2	B	602	STI	C50-C49-N48	2.41	115.58	110.64
2	A	601	STI	C18-C19-C14	2.25	119.56	117.44
2	A	601	STI	C50-C49-N48	2.16	115.08	110.64
2	A	601	STI	C29-C23-C25	2.12	121.61	118.59
2	A	601	STI	C14-N13-C9	-2.12	123.22	129.60
5	B	603	GOL	C3-C2-C1	-2.11	103.50	111.70
2	A	601	STI	C52-C53-N48	2.09	114.93	110.64
2	B	602	STI	C12-C7-N8	-2.04	118.78	121.46
3	B	605	KWV	O3-C2-N4	-2.04	118.52	121.82
3	A	602	KWV	O3-C2-N4	-2.02	118.55	121.82

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	STI	C15-C14-N13-C9
2	B	602	STI	C15-C14-N13-C9
6	B	606	2PE	C14-C15-O16-C17
6	B	606	2PE	C21-C20-O19-C18

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Mol	Chain	Res	Type	Atoms
6	B	606	2PE	O4-C5-C6-O7
6	B	606	2PE	O13-C14-C15-O16
6	B	606	2PE	O22-C23-C24-O25
6	B	606	2PE	O19-C20-C21-O22
5	B	603	GOL	O1-C1-C2-O2
6	B	606	2PE	O10-C11-C12-O13
6	B	606	2PE	O1-C2-C3-O4
5	B	603	GOL	O1-C1-C2-C3
5	B	603	GOL	C1-C2-C3-O3
6	B	606	2PE	O25-C26-C27-O28
6	B	606	2PE	O7-C8-C9-O10
6	B	606	2PE	C8-C9-O10-C11
6	B	606	2PE	C12-C11-O10-C9
6	B	606	2PE	C11-C12-O13-C14
6	B	606	2PE	C17-C18-O19-C20
6	B	606	2PE	C9-C8-O7-C6
6	B	606	2PE	C27-C26-O25-C24
6	B	606	2PE	C24-C23-O22-C21
2	A	601	STI	C19-C14-N13-C9
5	B	603	GOL	O2-C2-C3-O3

There are no ring outliers.

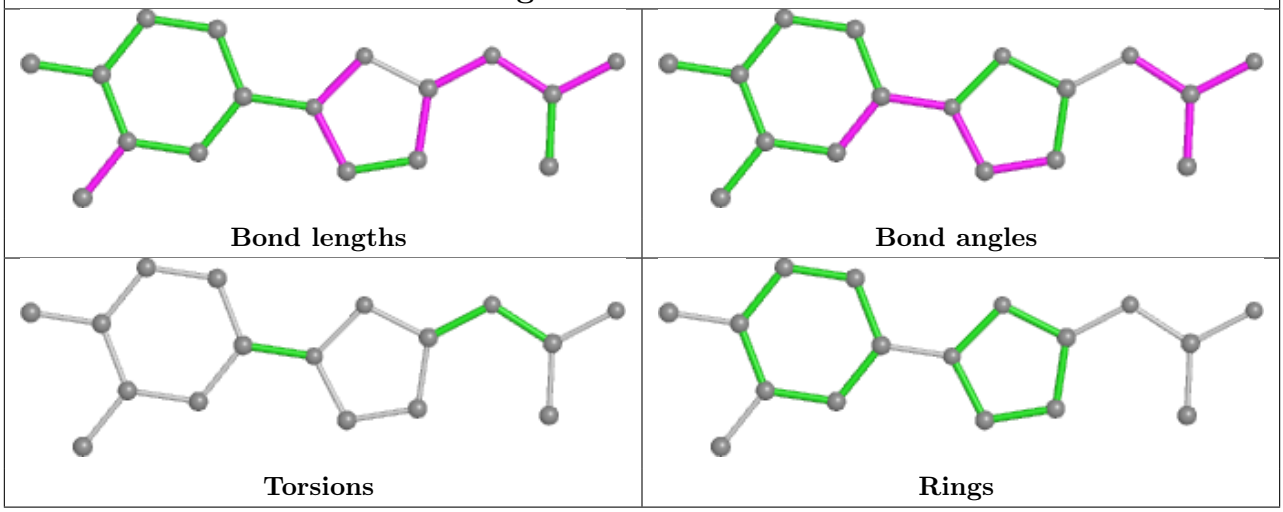
5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	605	KWV	3	0
5	B	603	GOL	2	0
2	A	601	STI	2	0
6	B	606	2PE	7	0
2	B	602	STI	2	0

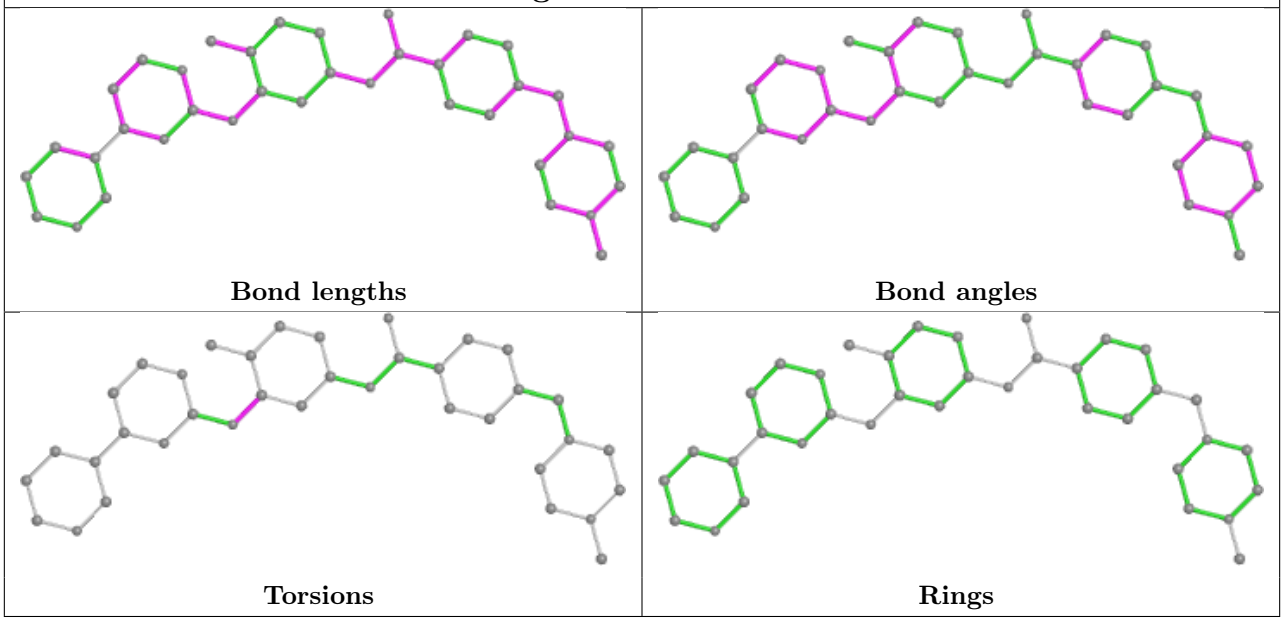
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

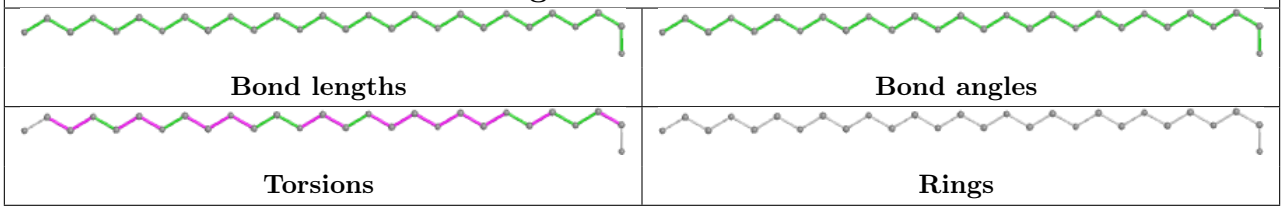
Ligand KWV B 605



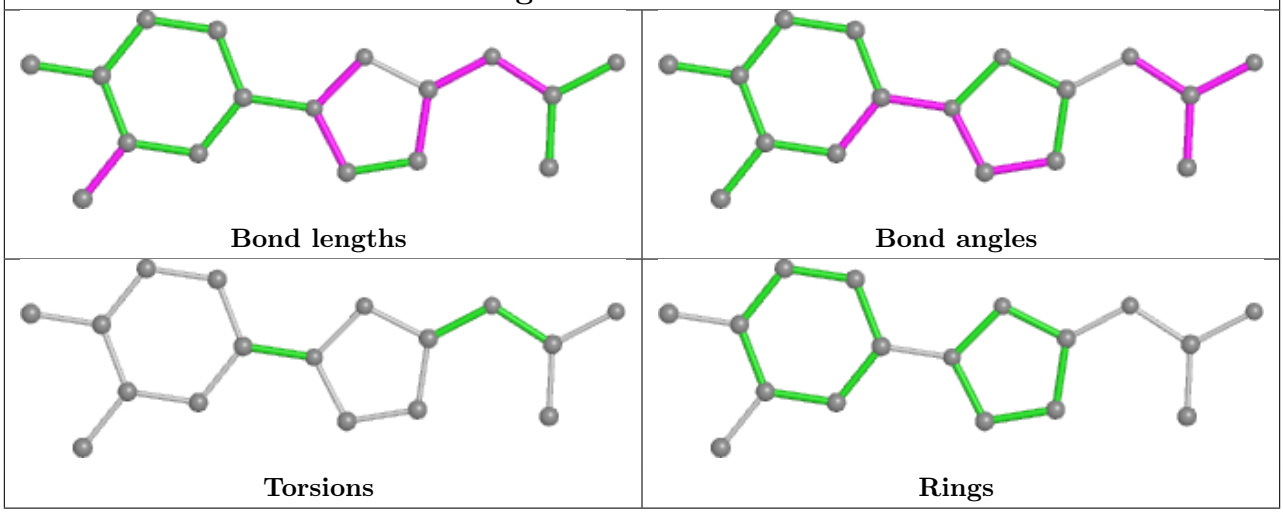
Ligand STI A 601



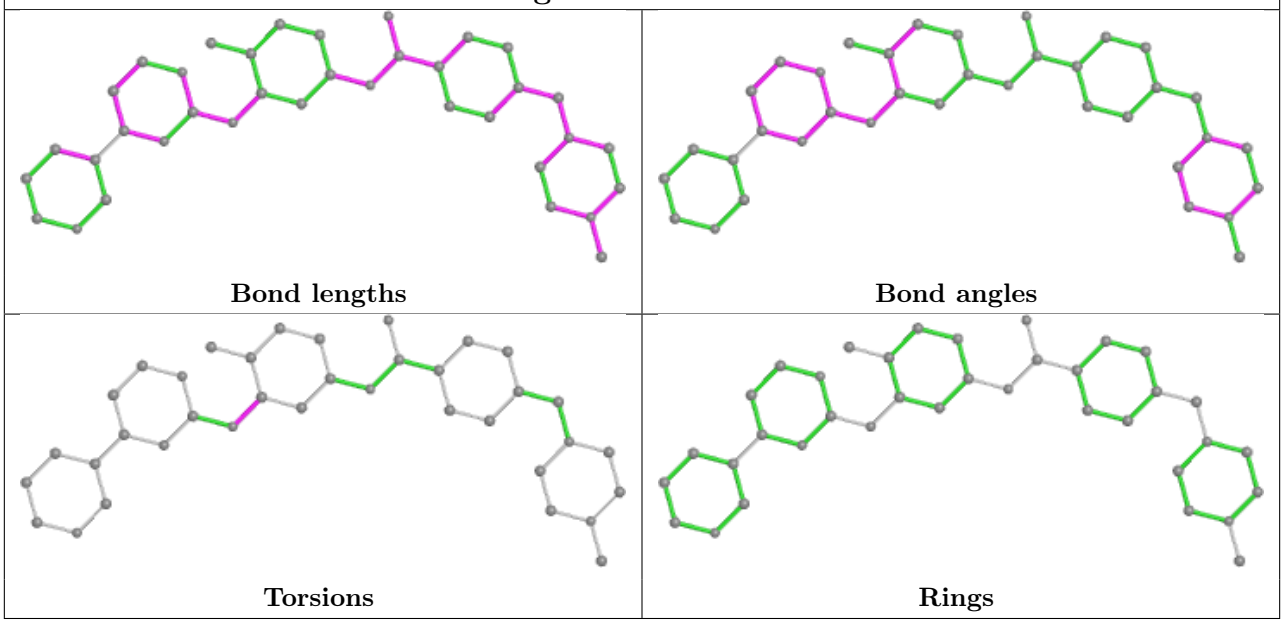
Ligand 2PE B 606



Ligand KWV A 602



Ligand STI B 602



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.11	6 (2%)	60	69	19, 29, 54, 72	0
1	B	257/298 (86%)	0.24	7 (2%)	54	64	20, 31, 70, 88	0
All	All	521/596 (87%)	0.17	13 (2%)	57	66	19, 30, 64, 88	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	420	PHE	6.9
1	B	418	ALA	5.1
1	A	418	ALA	3.7
1	B	419	LYS	3.6
1	A	417	GLY	3.3
1	A	416	ALA	3.2
1	B	292	LEU	2.6
1	A	406	LEU	2.5
1	A	405	ARG	2.4
1	B	330	PHE	2.4
1	B	329	PRO	2.4
1	A	293	LYS	2.1
1	B	268	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

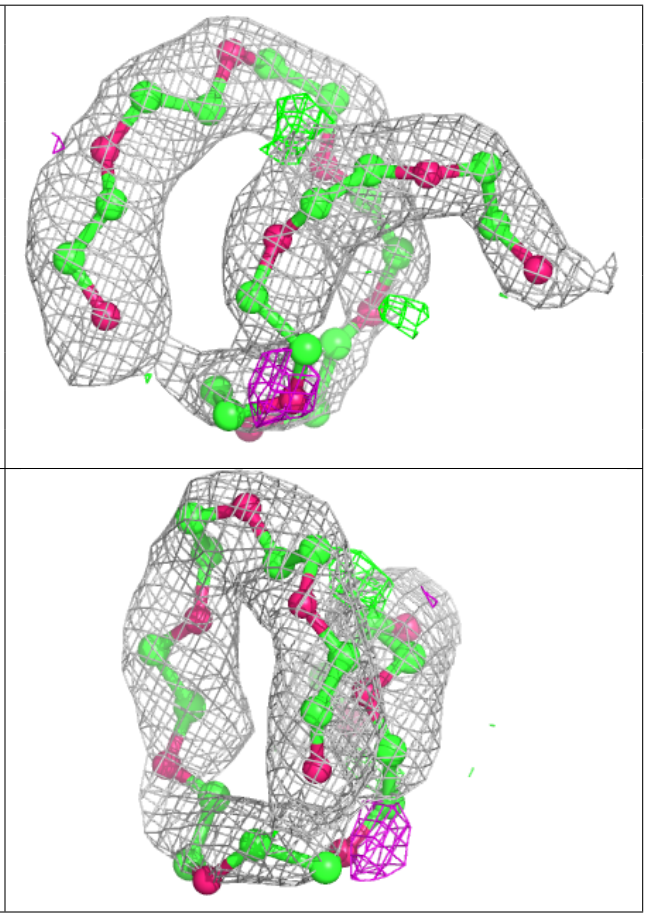
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	2PE	B	606	28/28	0.86	0.24	39,52,66,73	0
4	SO4	B	601	5/5	0.90	0.20	67,68,83,87	0
5	GOL	B	604	6/6	0.92	0.23	30,34,43,43	0
5	GOL	B	603	6/6	0.92	0.16	23,37,41,41	0
3	KWV	B	605	17/17	0.95	0.14	22,26,32,42	0
3	KWV	A	602	17/17	0.96	0.13	19,24,35,38	0
2	STI	A	601	37/37	0.97	0.15	19,24,34,37	0
2	STI	B	602	37/37	0.97	0.15	30,36,41,42	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.

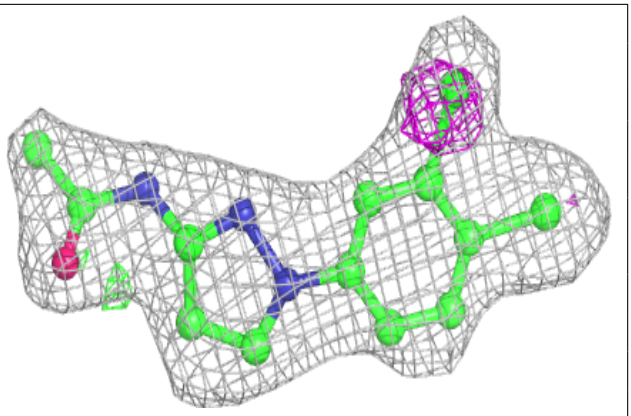
Electron density around 2PE B 606:

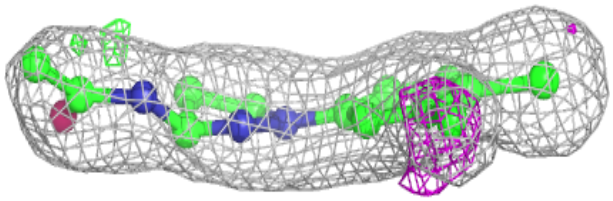
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

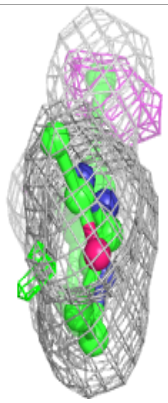


Electron density around KWV B 605:

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

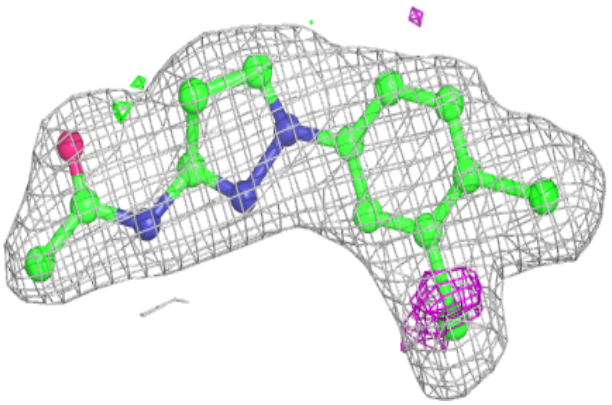


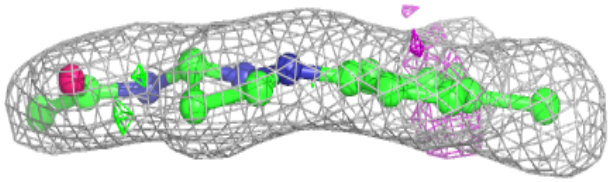


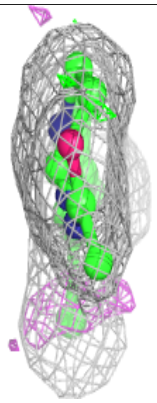


Electron density around KWV A 602:

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

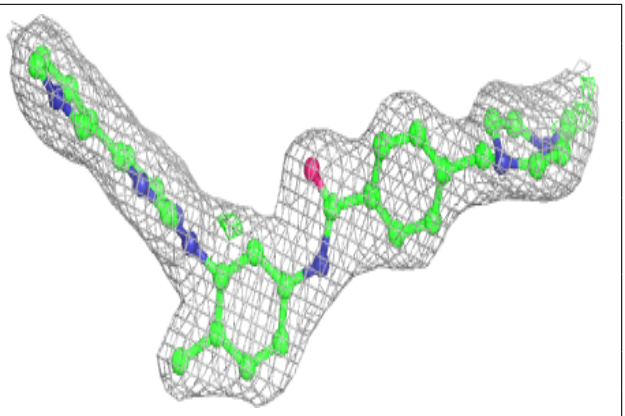


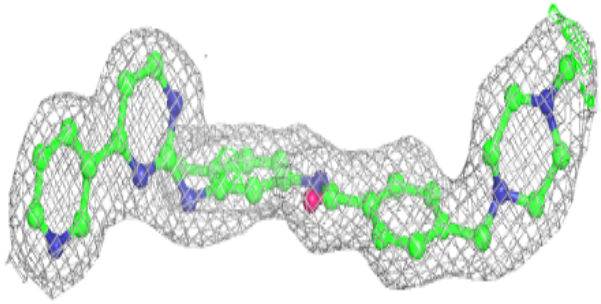


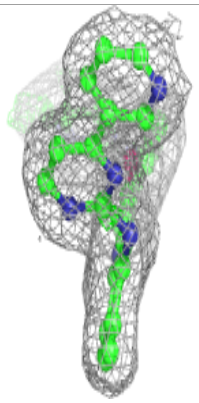


Electron density around STI A 601:

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

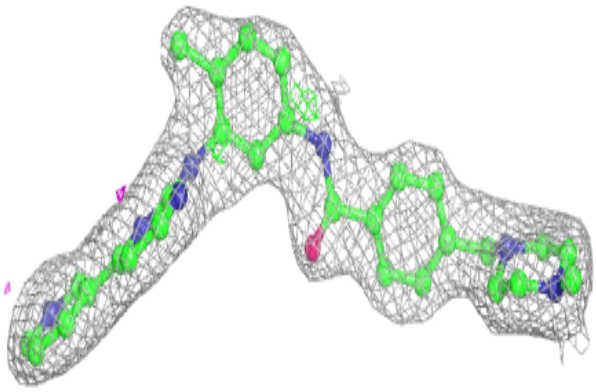


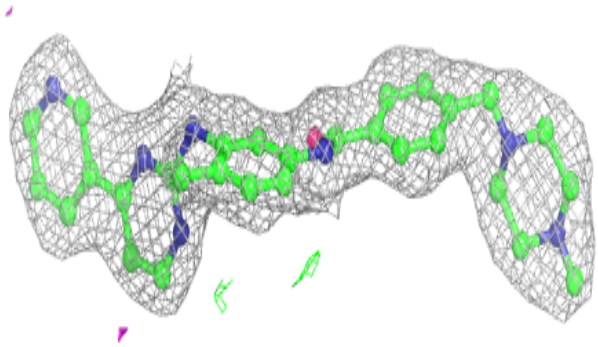


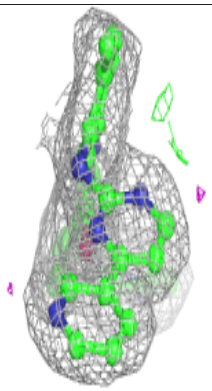


Electron density around STI B 602:

$2mF_o$-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 (i)

There are no such residues in this entry.