



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:36 PM UTC

PDB ID : 7S4C / pdb_00007s4c
Title : Crystal Structure of Inhibitor-bound Galactokinase
Authors : Whitby, F.G.
Deposited on : 2021-09-08
Resolution : 2.20 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

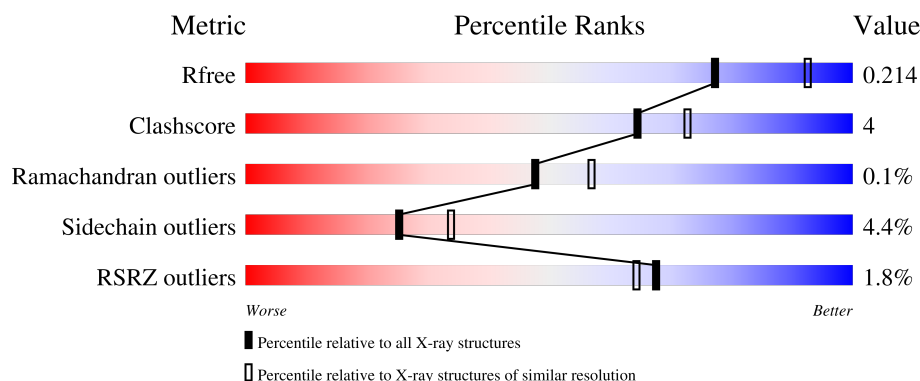
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	392	2% 90% 9%
1	B	392	2% 84% 14%

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
3	V3V	A	403	X	-	-	-
5	PO4	B	404	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12513 atoms, of which 5972 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.

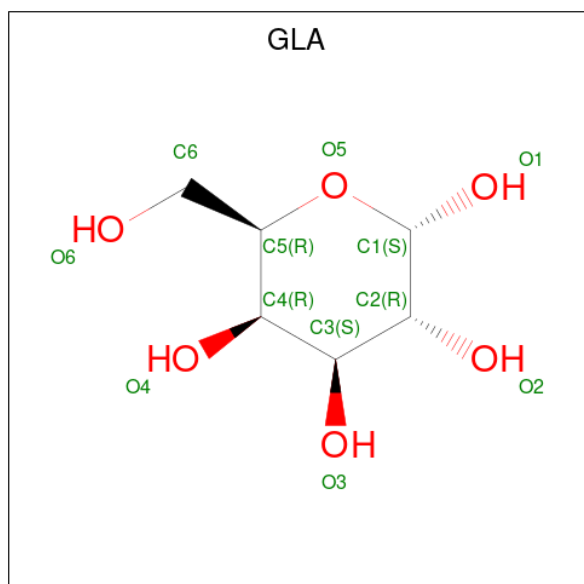
- Molecule 1 is a protein called Galactokinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	391	5909	1846	2951	535	560	17	0	1	0
1	B	391	5896	1841	2946	534	559	16	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

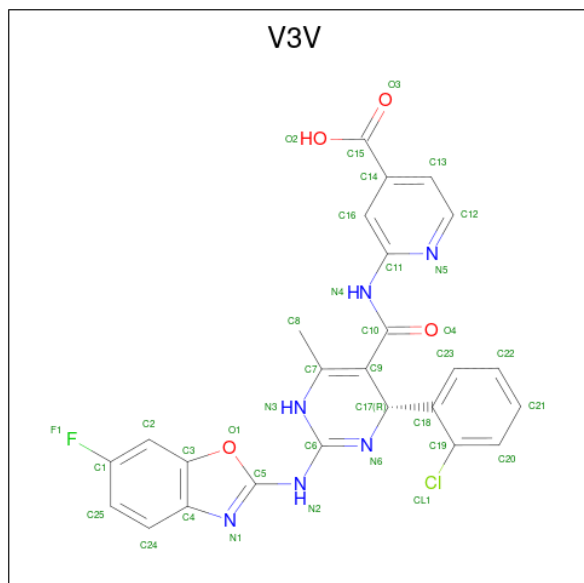
Chain	Residue	Modelled	Actual	Comment	Reference
A	252	ALA	LYS	engineered mutation	UNP P51570
A	253	ALA	GLU	engineered mutation	UNP P51570
B	252	ALA	LYS	engineered mutation	UNP P51570
B	253	ALA	GLU	engineered mutation	UNP P51570

- Molecule 2 is alpha-D-galactopyranose (CCD ID: GLA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			24	6	12	6		
2	B	1	Total	C	H	O	0	0
			24	6	12	6		

- Molecule 3 is 2-((4R)-4-(2-chlorophenyl)-2-[(6-fluoro-1,3-benzoxazol-2-yl)amino]-6-methyl-1,4-dihydropyrimidine-5-carbonyl)amino)pyridine-4-carboxylic acid (CCD ID: V3V) (formula: C₂₅H₁₈ClFN₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	H	N	O	0	0
			54	25	1	1	17	6	4		
3	A	1	Total	C	Cl	F	H	N	O	0	0
			54	25	1	1	17	6	4		
3	B	1	Total	C	Cl	F	H	N	O	0	0
			54	25	1	1	17	6	4		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

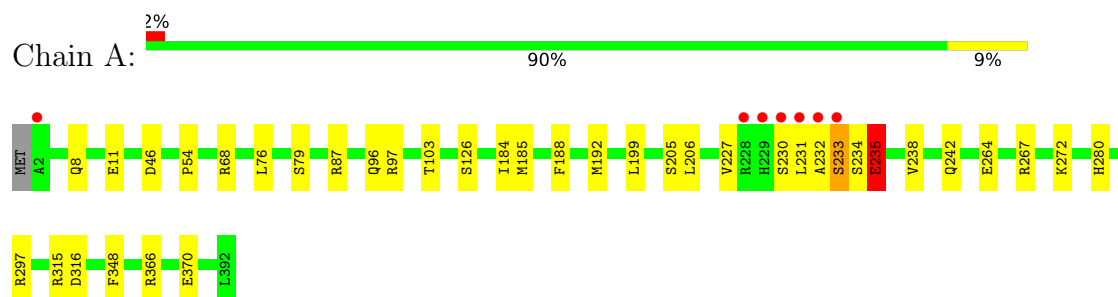
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	268	Total	O	0	0
			268	268		
6	B	208	Total	O	0	0
			208	208		

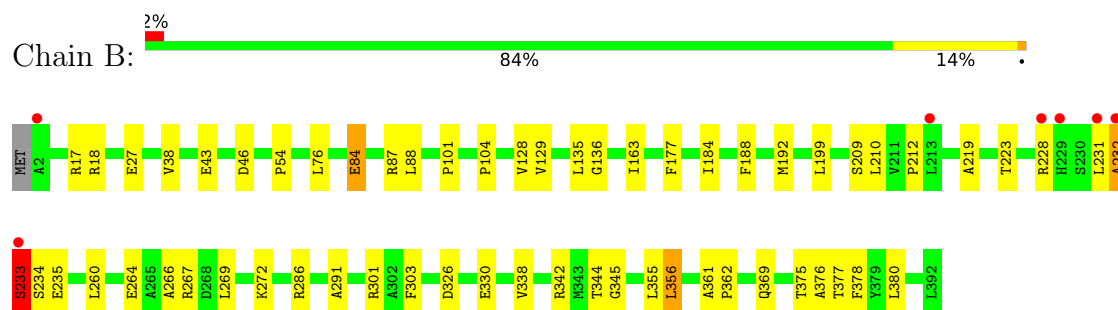
3 Residue-property plots [i](#)

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: Galactokinase



- Molecule 1: Galactokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	129.22Å 129.22Å 240.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.61 – 2.20 38.61 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.61-2.20) 99.9 (38.61-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.176 , 0.215 0.176 , 0.214	Depositor DCC
R_{free} test set	2268 reflections (3.45%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12513	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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: NA, GLA, V3V, PO4

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	0.77	1/3012 (0.0%)	1.13	4/4084 (0.1%)
1	B	0.72	0/3004	1.10	5/4074 (0.1%)
All	All	0.74	1/6016 (0.0%)	1.12	9/8158 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	GLU	CD-OE1	5.27	1.35	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	ASP	CA-CB-CG	6.83	119.43	112.60
1	A	97	ARG	CB-CA-C	-5.98	100.58	110.14
1	A	280	HIS	CA-CB-CG	-5.84	107.96	113.80
1	B	84	GLU	CB-CG-CD	5.63	122.18	112.60
1	A	235	GLU	CB-CG-CD	5.42	121.81	112.60
1	A	46	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	87	ARG	CB-CA-C	-5.22	99.81	109.37
1	B	345	GLY	CA-C-N	5.05	125.59	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	GLY	C-N-CA	5.05	125.59	119.98

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	ALA	Peptide
1	A	233	SER	Peptide
1	B	232	ALA	Peptide

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	2958	2951	2953	17	0
1	B	2950	2946	2945	29	1
2	A	12	12	12	0	0
2	B	12	12	12	0	0
3	A	74	34	0	0	0
3	B	37	17	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	15	0	0	0	0
5	B	5	0	0	2	0
6	A	268	0	0	0	0
6	B	208	0	0	0	0
All	All	6541	5972	5922	47	1

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 (47) 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:231:LEU:HD22	1:A:235:GLU:HG2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ARG:NH1	1:B:27:GLU:OE1	2.27	0.67
1:A:231:LEU:HA	1:A:234:SER:HB3	1.78	0.65
1:B:199:LEU:CD1	1:B:210:LEU:HD23	2.28	0.64
1:B:231:LEU:HA	1:B:234:SER:HB3	1.82	0.62
1:B:260:LEU:O	1:B:264:GLU:HG3	2.02	0.59
1:B:356:LEU:HD12	1:B:356:LEU:N	2.19	0.58
1:A:230:SER:O	1:A:231:LEU:HG	2.04	0.57
1:A:231:LEU:HD13	1:A:348:PHE:CD1	2.40	0.57
1:B:199:LEU:HD12	1:B:210:LEU:HD23	1.86	0.56
1:B:136:GLY:HA2	5:B:404:PO4:O2	2.09	0.52
1:B:136:GLY:HA2	5:B:404:PO4:P	2.50	0.51
1:A:54:PRO:HD2	1:A:199:LEU:O	2.10	0.51
1:A:188:PHE:CE2	1:A:192[B]:MET:HE1	2.46	0.50
1:A:230:SER:C	1:A:231:LEU:HG	2.36	0.50
1:B:223:THR:HG23	1:B:378:PHE:CE1	2.47	0.49
1:B:76:LEU:O	1:B:128:VAL:HA	2.12	0.49
1:A:366:ARG:O	1:A:370:GLU:HG3	2.13	0.49
1:A:231:LEU:CD2	1:A:235:GLU:HG2	2.39	0.48
1:B:163:ILE:CG2	1:B:192:MET:HE2	2.44	0.48
1:B:163:ILE:HG21	1:B:192:MET:HE2	1.96	0.47
1:B:338:VAL:HA	1:B:356:LEU:HB3	1.96	0.47
1:A:205:SER:O	1:A:206:LEU:HB2	2.14	0.47
1:B:38:VAL:HG23	1:B:344:THR:HG21	1.96	0.46
1:B:54:PRO:HD2	1:B:199:LEU:O	2.15	0.46
1:A:238:VAL:O	1:A:242:GLN:HG3	2.16	0.46
1:B:369:GLN:HE22	1:B:376:ALA:H	1.62	0.46
1:B:266:ALA:HB1	1:B:269:LEU:HD12	1.97	0.45
3:B:402:V3V:N1	3:B:402:V3V:N6	2.64	0.45
1:B:188:PHE:CE1	1:B:192:MET:HG3	2.51	0.44
1:A:76:LEU:C	1:A:76:LEU:HD23	2.42	0.44
1:A:188:PHE:CD2	1:A:192[B]:MET:SD	3.11	0.44
1:B:43:GLU:HB2	1:B:342:ARG:NH2	2.33	0.43
1:B:101:PRO:HG3	1:B:177:PHE:HA	1.99	0.43
1:B:219:ALA:HB3	1:B:356:LEU:HD13	2.00	0.43
1:A:68:ARG:HD2	1:A:126:SER:OG	2.19	0.43
1:B:291:ALA:HB1	1:B:303:PHE:CE2	2.54	0.43
1:B:361:ALA:HB3	1:B:362:PRO:HD3	2.01	0.42
1:B:88:LEU:HD12	1:B:88:LEU:HA	1.85	0.42
1:B:380:LEU:HD12	1:B:380:LEU:HA	1.84	0.42
1:A:184:ILE:O	1:A:185:MET:C	2.63	0.41
1:A:231:LEU:C	1:A:234:SER:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:HD22	1:B:104:PRO:HD2	2.03	0.41
1:B:228:ARG:HD2	1:B:228:ARG:HA	1.89	0.41
1:B:326:ASP:O	1:B:330:GLU:HG2	2.21	0.40
1:A:315:ARG:HD2	1:A:316:ASP:OD1	2.21	0.40
1:B:232:ALA:O	1:B:233:SER:C	2.65	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ARG:HH12	1:B:235:GLU:OE1[5_554]	1.56	0.04

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	390/392 (100%)	382 (98%)	8 (2%)	0	100	100
1	B	389/392 (99%)	377 (97%)	11 (3%)	1 (0%)	36	42
All	All	779/784 (99%)	759 (97%)	19 (2%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	233	SER

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	309/309 (100%)	297 (96%)	12 (4%)	28	39
1	B	308/309 (100%)	293 (95%)	15 (5%)	22	29
All	All	617/618 (100%)	590 (96%)	27 (4%)	25	34

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	79	SER
1	A	87	ARG
1	A	96	GLN
1	A	103	THR
1	A	227	VAL
1	A	233	SER
1	A	235	GLU
1	A	264	GLU
1	A	267	ARG
1	A	272	LYS
1	A	297	ARG
1	B	84	GLU
1	B	129	VAL
1	B	135	LEU
1	B	184	ILE
1	B	209	SER
1	B	212	PRO
1	B	233	SER
1	B	267	ARG
1	B	272	LYS
1	B	286	ARG
1	B	301	ARG
1	B	355	LEU
1	B	356	LEU
1	B	375	THR
1	B	377	THR

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	89	GLN

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Mol	Chain	Res	Type
1	A	229	HIS
1	A	382	GLN
1	B	327	GLN
1	B	367	HIS
1	B	371	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 for Mogul analysis.

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	V3V	A	403	-	40,41,41	3.28	24 (60%)	51,59,59	2.83	21 (41%)
3	V3V	B	402	-	40,41,41	2.09	9 (22%)	51,59,59	2.14	18 (35%)
5	PO4	A	406	-	4,4,4	0.75	0	6,6,6	0.49	0
5	PO4	A	405	-	4,4,4	1.08	0	6,6,6	0.67	0
5	PO4	A	407	-	4,4,4	0.72	0	6,6,6	0.48	0
3	V3V	A	402	-	40,41,41	1.56	11 (27%)	51,59,59	1.96	14 (27%)
5	PO4	B	404	-	4,4,4	1.67	1 (25%)	6,6,6	0.28	0
2	GLA	A	401	-	12,12,12	1.01	0	17,17,17	1.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLA	B	401	-	12,12,12	0.73	0	17,17,17	1.20	2 (11%)

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	V3V	A	403	-	1/1/9/9	11/20/36/36	0/5/5/5
3	V3V	B	402	-	-	4/20/36/36	0/5/5/5
3	V3V	A	402	-	-	4/20/36/36	0/5/5/5
2	GLA	A	401	-	-	1/2/22/22	0/1/1/1
2	GLA	B	401	-	-	1/2/22/22	0/1/1/1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	V3V	C7-C9	8.37	1.45	1.35
3	B	402	V3V	C5-N1	6.31	1.41	1.30
3	B	402	V3V	C17-N6	-5.93	1.41	1.47
3	A	403	V3V	C5-N1	5.73	1.40	1.30
3	A	403	V3V	C10-N4	5.56	1.47	1.35
3	B	402	V3V	C7-C9	5.35	1.42	1.35
3	A	403	V3V	C18-C17	5.00	1.59	1.52
3	A	403	V3V	C10-C9	4.59	1.54	1.49
3	A	403	V3V	C17-N6	-4.38	1.42	1.47
3	A	403	V3V	C19-C18	4.38	1.44	1.39
3	A	402	V3V	C17-N6	-4.36	1.42	1.47
3	A	403	V3V	C14-C15	4.33	1.58	1.49
3	A	403	V3V	C6-N3	4.05	1.43	1.36
3	A	403	V3V	C23-C18	3.90	1.44	1.39
3	A	403	V3V	C2-C1	3.76	1.43	1.37
3	A	403	V3V	O1-C5	3.68	1.44	1.37
3	A	403	V3V	O3-C15	3.68	1.33	1.22
3	A	403	V3V	C13-C14	3.32	1.44	1.39
3	B	402	V3V	C8-C7	3.19	1.55	1.49
3	A	403	V3V	C16-C14	3.10	1.44	1.39
5	B	404	PO4	P-O1	3.08	1.57	1.50
3	A	403	V3V	C19-CL1	2.90	1.80	1.73
3	A	403	V3V	C3-C4	2.89	1.42	1.38
3	B	402	V3V	C10-N4	2.81	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	V3V	C5-N2	2.78	1.41	1.36
3	A	403	V3V	C8-C7	2.73	1.54	1.49
3	A	403	V3V	C22-C23	2.73	1.43	1.38
3	A	403	V3V	C25-C1	2.70	1.42	1.37
3	A	403	V3V	C13-C12	2.67	1.43	1.38
3	B	402	V3V	C19-CL1	2.62	1.79	1.73
3	A	402	V3V	C25-C1	2.61	1.42	1.37
3	A	403	V3V	C20-C19	2.58	1.44	1.38
3	A	402	V3V	C8-C7	2.55	1.54	1.49
3	A	402	V3V	C19-C18	-2.51	1.36	1.39
3	A	402	V3V	C10-N4	2.45	1.40	1.35
3	A	403	V3V	O1-C3	2.45	1.42	1.38
3	B	402	V3V	C22-C23	2.42	1.43	1.38
3	A	402	V3V	C5-N1	2.38	1.34	1.30
3	A	402	V3V	C7-C9	2.27	1.38	1.35
3	A	402	V3V	C23-C18	2.20	1.42	1.39
3	A	402	V3V	O2-C15	-2.16	1.24	1.30
3	A	402	V3V	C13-C12	2.10	1.42	1.38
3	B	402	V3V	C3-C4	2.08	1.41	1.38
3	A	402	V3V	C18-C17	2.05	1.55	1.52
3	B	402	V3V	C10-C9	-2.04	1.46	1.49

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	V3V	C9-C7-N3	-9.12	111.64	119.29
3	A	403	V3V	C8-C7-N3	7.25	121.86	113.42
3	B	402	V3V	C9-C7-N3	-7.07	113.36	119.29
3	A	403	V3V	C2-C3-C4	-6.39	117.86	124.45
3	A	403	V3V	C18-C17-N6	6.20	119.17	109.22
3	A	402	V3V	C9-C7-N3	-6.12	114.16	119.29
3	A	402	V3V	N2-C6-N3	-5.00	109.55	117.96
3	B	402	V3V	C12-N5-C11	4.49	123.63	117.21
3	A	402	V3V	N2-C6-N6	4.48	126.22	117.95
3	A	403	V3V	O1-C3-C2	4.23	133.86	124.95
3	A	403	V3V	O4-C10-C9	-4.16	113.79	121.32
3	A	403	V3V	O1-C5-N1	-4.15	108.11	115.57
3	B	402	V3V	C8-C7-N3	3.83	117.88	113.42
3	A	402	V3V	O1-C5-N1	-3.74	108.84	115.57
3	A	403	V3V	C16-C11-N5	-3.73	118.02	122.92
3	A	402	V3V	C11-N4-C10	-3.56	122.91	128.06
3	A	403	V3V	C12-N5-C11	3.47	122.17	117.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	V3V	N2-C6-N3	-3.41	112.23	117.96
3	A	403	V3V	C13-C14-C16	-3.35	115.37	119.25
3	A	403	V3V	N2-C5-N1	-3.29	119.25	128.58
3	B	402	V3V	N2-C6-N6	3.28	124.00	117.95
3	B	402	V3V	C11-N4-C10	-3.26	123.35	128.06
3	B	402	V3V	C18-C19-CL1	-3.17	117.17	120.41
3	A	402	V3V	O1-C3-C2	3.00	131.26	124.95
3	A	403	V3V	C9-C10-N4	2.92	120.57	116.01
3	B	402	V3V	C13-C12-N5	-2.92	120.39	123.97
3	B	402	V3V	C5-N2-C6	-2.90	118.17	125.27
3	A	403	V3V	C14-C16-C11	2.90	122.99	118.45
3	A	403	V3V	C5-N2-C6	2.90	132.36	125.27
3	B	402	V3V	C24-C25-C1	2.82	121.27	118.38
3	A	402	V3V	C12-N5-C11	2.68	121.04	117.21
2	B	401	GLA	O1-C1-C2	-2.60	101.43	108.98
3	B	402	V3V	C12-C13-C14	-2.57	116.24	119.05
3	B	402	V3V	O1-C5-N1	-2.55	110.98	115.57
3	B	402	V3V	C10-C9-C7	-2.52	117.43	123.25
3	A	403	V3V	C13-C12-N5	-2.51	120.89	123.97
3	A	403	V3V	C24-C4-C3	2.50	123.50	120.31
3	A	403	V3V	C4-N1-C5	2.50	109.08	104.13
3	B	402	V3V	C16-C11-N5	-2.44	119.72	122.92
3	A	402	V3V	O1-C3-C4	-2.39	106.17	107.80
2	B	401	GLA	C1-O5-C5	2.36	118.22	113.65
3	A	403	V3V	O3-C15-C14	2.35	127.61	121.46
3	A	402	V3V	C13-C12-N5	-2.31	121.14	123.97
3	B	402	V3V	C13-C14-C16	2.26	121.86	119.25
3	B	402	V3V	C19-C18-C17	-2.24	117.70	121.98
3	A	402	V3V	C8-C7-N3	2.17	115.94	113.42
3	A	402	V3V	C5-N2-C6	-2.16	119.99	125.27
3	B	402	V3V	O2-C15-C14	2.13	120.31	114.84
3	A	403	V3V	C16-C14-C15	2.13	123.77	119.96
3	A	403	V3V	C17-C9-C7	-2.10	116.27	120.94
3	A	402	V3V	O2-C15-O3	-2.08	118.89	123.35
3	A	402	V3V	C8-C7-C9	2.08	129.68	127.61
3	B	402	V3V	O1-C3-C2	2.01	129.18	124.95
3	A	403	V3V	C18-C19-CL1	-2.01	118.36	120.41
3	A	402	V3V	C9-C10-N4	-2.01	112.87	116.01

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
3	A	403	V3V	C17

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	V3V	N3-C6-N2-C5
3	A	403	V3V	N6-C6-N2-C5
3	A	403	V3V	N1-C5-N2-C6
3	A	403	V3V	O1-C5-N2-C6
3	B	402	V3V	N5-C11-N4-C10
3	A	402	V3V	N5-C11-N4-C10
3	B	402	V3V	C16-C11-N4-C10
3	A	402	V3V	C16-C11-N4-C10
2	B	401	GLA	O5-C5-C6-O6
2	A	401	GLA	O5-C5-C6-O6
3	A	402	V3V	N3-C6-N2-C5
3	A	402	V3V	N6-C6-N2-C5
3	B	402	V3V	N6-C6-N2-C5
3	A	403	V3V	C16-C14-C15-O3
3	A	403	V3V	N4-C10-C9-C17
3	A	403	V3V	O4-C10-C9-C7
3	A	403	V3V	N4-C10-C9-C7
3	B	402	V3V	N3-C6-N2-C5
3	A	403	V3V	C16-C14-C15-O2
3	A	403	V3V	C13-C14-C15-O3
3	A	403	V3V	C13-C14-C15-O2

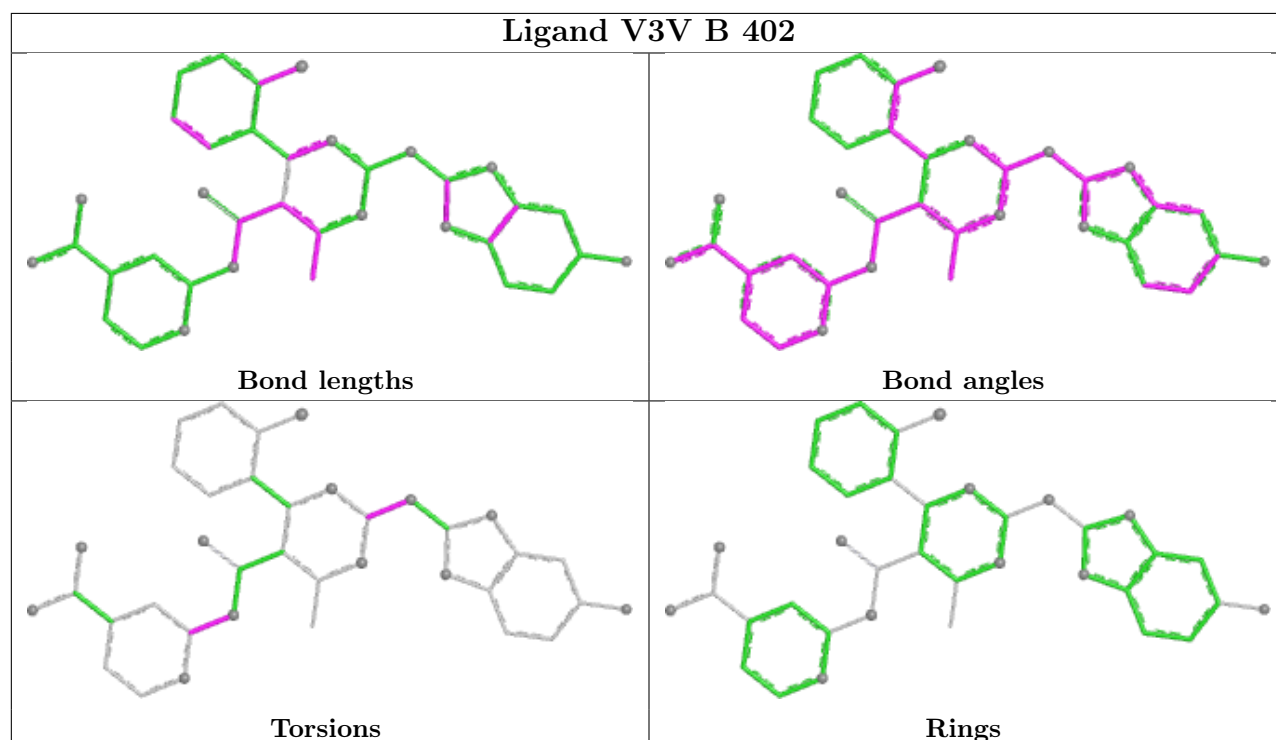
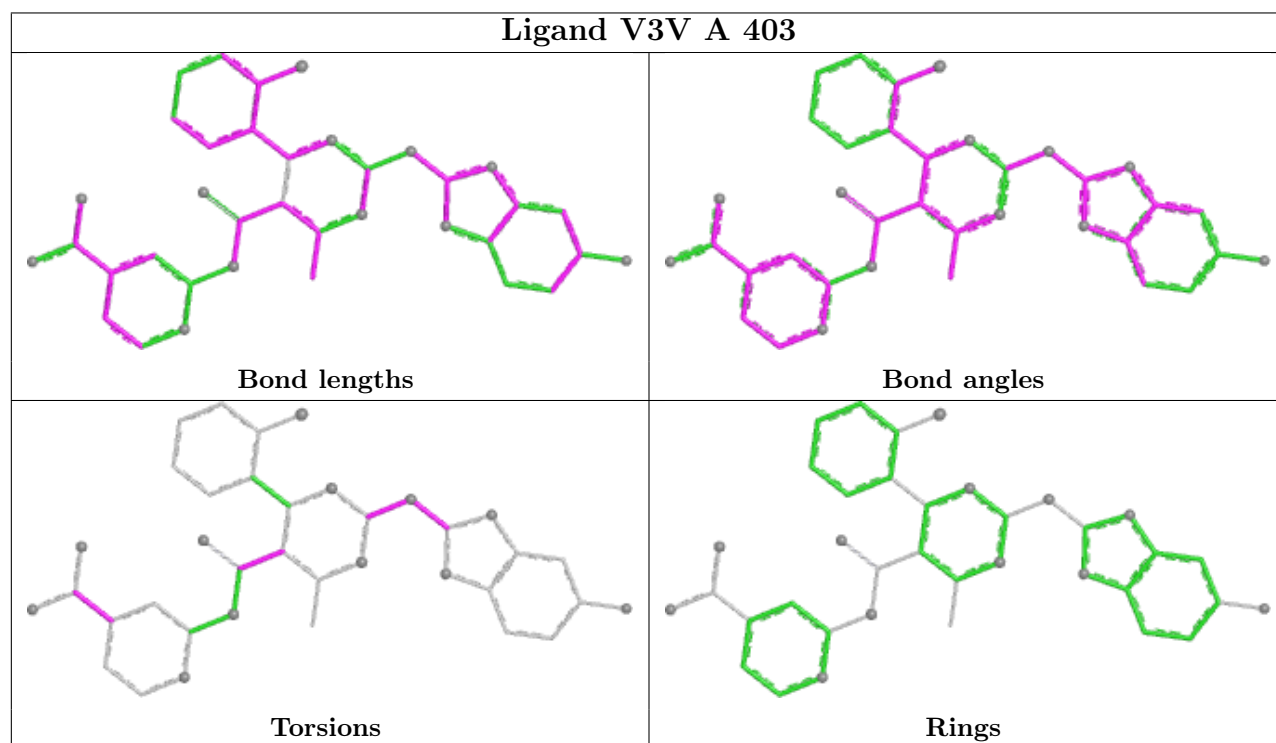
There are no ring outliers.

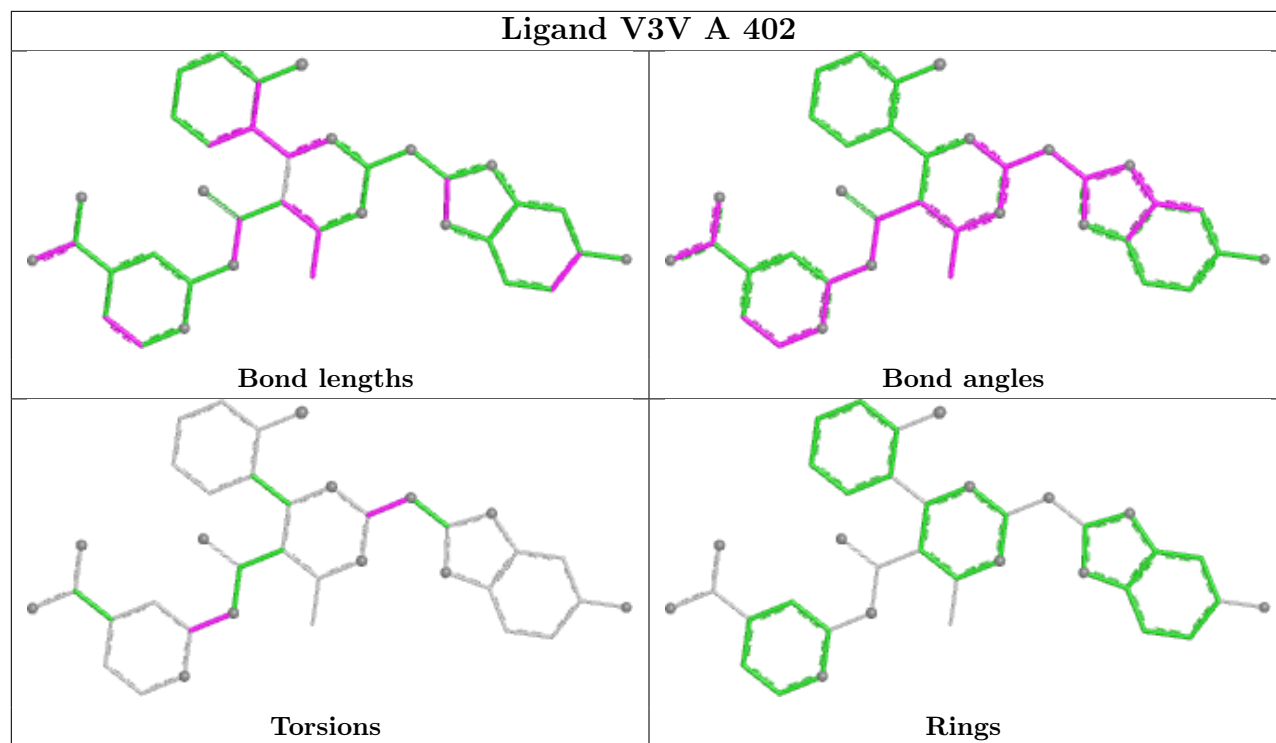
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	V3V	1	0
5	B	404	PO4	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 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 [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	391/392 (99%)	-0.49	7 (1%) 67 64	17, 37, 61, 117	1 (0%)
1	B	391/392 (99%)	-0.23	7 (1%) 67 64	23, 45, 85, 107	0
All	All	782/784 (99%)	-0.36	14 (1%) 67 64	17, 41, 80, 117	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	ALA	8.5
1	A	231	LEU	3.7
1	A	230	SER	3.5
1	A	229	HIS	3.2
1	A	233	SER	3.0
1	B	228	ARG	3.0
1	B	2	ALA	2.8
1	B	213	LEU	2.8
1	A	228	ARG	2.6
1	B	233	SER	2.6
1	B	232	ALA	2.5
1	B	229	HIS	2.2
1	B	231	LEU	2.1
1	A	2	ALA	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

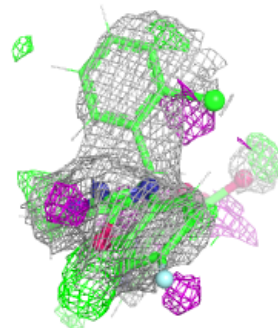
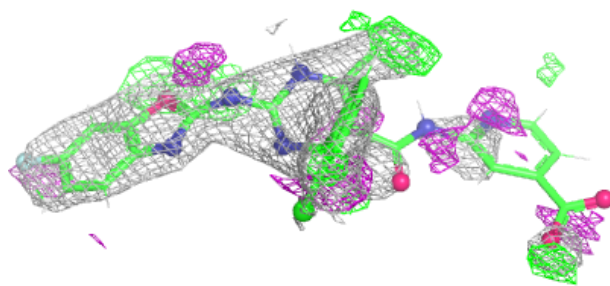
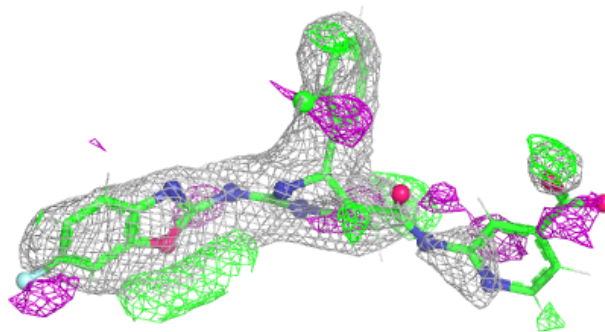
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	V3V	A	403	37/37	0.75	0.24	72,82,95,100	0
5	PO4	B	404	5/5	0.77	0.17	68,70,84,85	0
5	PO4	A	406	5/5	0.86	0.09	82,84,87,91	0
5	PO4	A	407	5/5	0.91	0.08	82,88,92,97	0
5	PO4	A	405	5/5	0.91	0.12	49,55,69,70	0
4	NA	B	403	1/1	0.92	0.08	77,77,77,77	0
3	V3V	A	402	37/37	0.97	0.07	29,36,51,67	0
4	NA	A	404	1/1	0.98	0.09	35,35,35,35	0
3	V3V	B	402	37/37	0.98	0.06	35,41,53,59	0
2	GLA	B	401	12/12	0.99	0.04	26,30,32,34	0
2	GLA	A	401	12/12	0.99	0.03	28,29,33,34	0

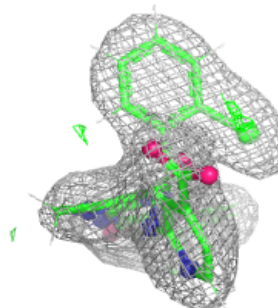
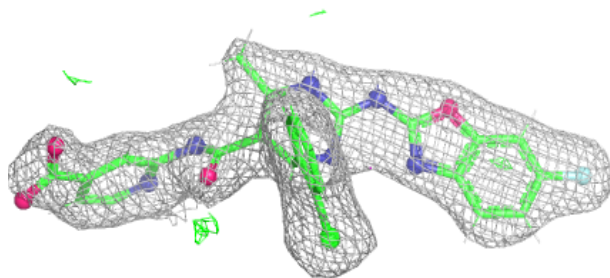
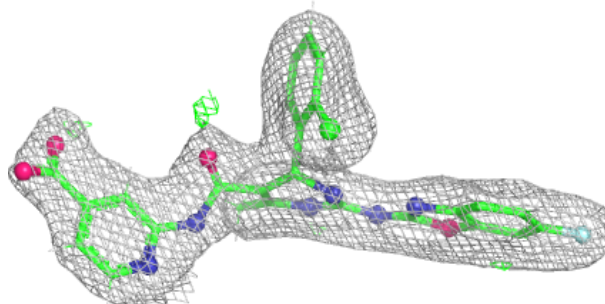
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around V3V A 403:

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

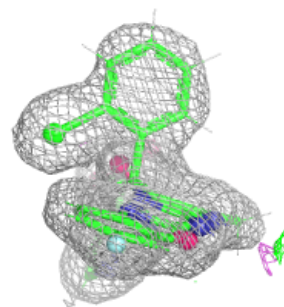
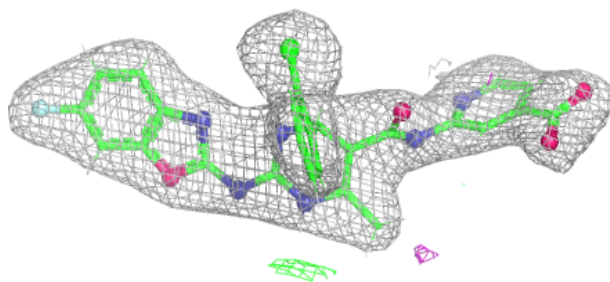
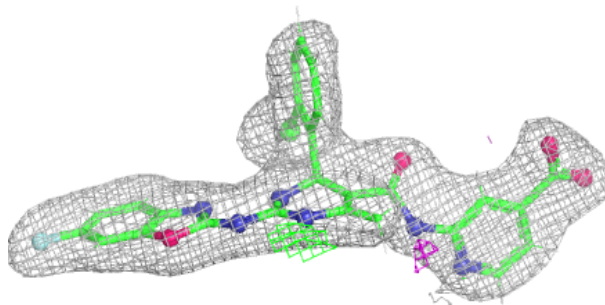
**Electron density around V3V A 402:**

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



Electron density around V3V B 402:

$2mF_o-DF_c$ (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.