



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:07 PM UTC

PDB ID : 7ONK / pdb_00007onk
Title : Crystal structure of PBP3 from *P. aeruginosa* in complex with AIC499
Authors : Freischem, S.; Grimm, I.; Weiergraeber, O.H.
Deposited on : 2021-05-25
Resolution : 1.73 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

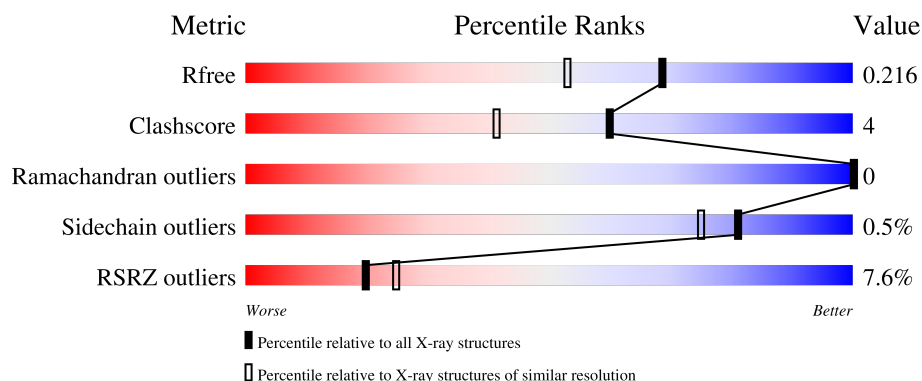
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	531	8% 86% 10% .
1	B	531	6% 88% 7% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8813 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.

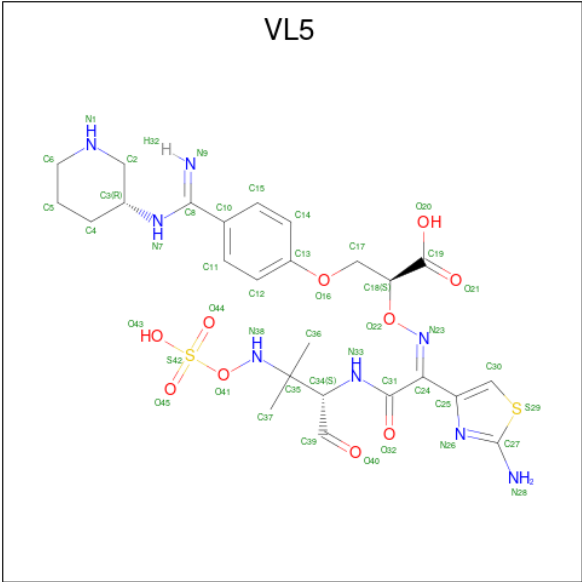
- Molecule 1 is a protein called Peptidoglycan D,D-transpeptidase FtsI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	18	0
			3962	2502	722	726	12			
1	B	505	Total	C	N	O	S	0	16	0
			3841	2426	683	720	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	MET	-	initiating methionine	UNP G3XD46
A	564	LYS	-	expression tag	UNP G3XD46
A	565	LEU	-	expression tag	UNP G3XD46
A	566	VAL	-	expression tag	UNP G3XD46
A	567	PRO	-	expression tag	UNP G3XD46
A	568	ARG	-	expression tag	UNP G3XD46
A	569	GLY	-	expression tag	UNP G3XD46
B	39	MET	-	initiating methionine	UNP G3XD46
B	564	LYS	-	expression tag	UNP G3XD46
B	565	LEU	-	expression tag	UNP G3XD46
B	566	VAL	-	expression tag	UNP G3XD46
B	567	PRO	-	expression tag	UNP G3XD46
B	568	ARG	-	expression tag	UNP G3XD46
B	569	GLY	-	expression tag	UNP G3XD46

- Molecule 2 is (2S)-2-[(Z)-[1-(2-azanyl-1,3-thiazol-4-yl)-2-[[[(2S)-3-methyl-1-oxidanylidene-3-(sulfooxyamino)butan-2-yl]amino]-2-oxidanylidene-ethylidene]amino]oxy-3-[4-[N-[(3R)-piperidin-3-yl]carbamidoyl]phenoxy]propanoic acid (CCD ID: VL5) (formula: C₂₅H₃₄N₈O₁₀S₂) (labeled as "Ligand of Interest" by depositor).

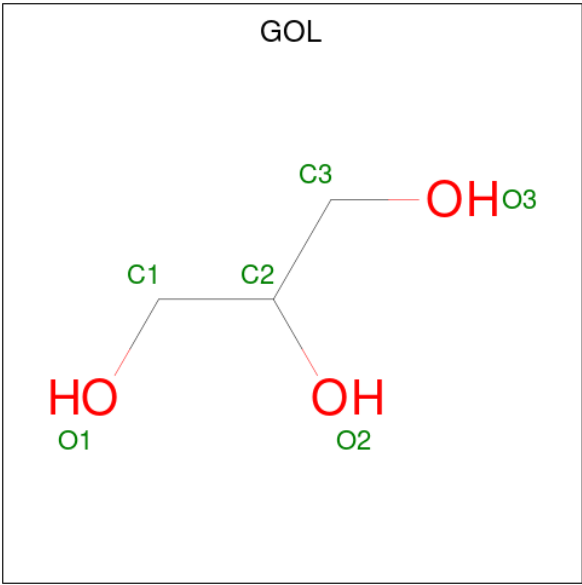


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 90	C 50	N 16	O 20	S 4	0	1
2	B	1	Total 90	C 50	N 16	O 20	S 4	0	1

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

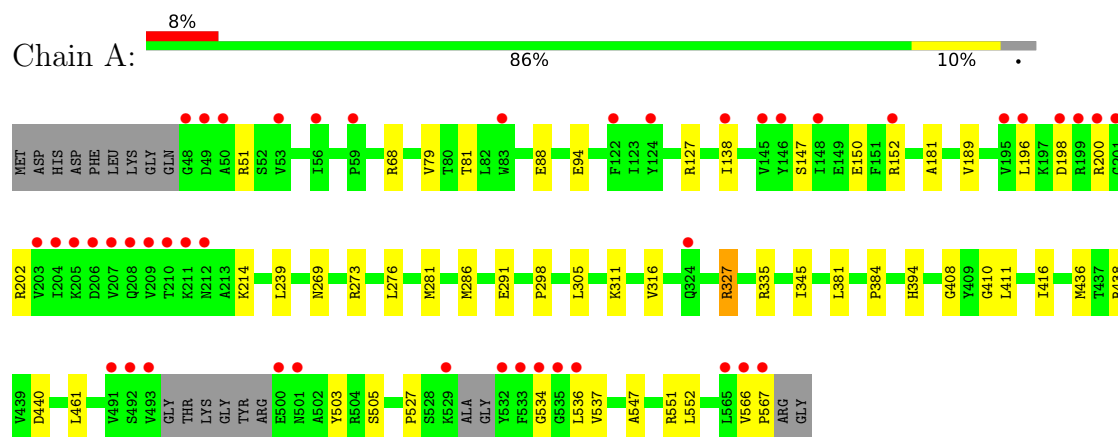
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	419	Total O 419 419	0	0
5	B	331	Total O 331 331	0	0

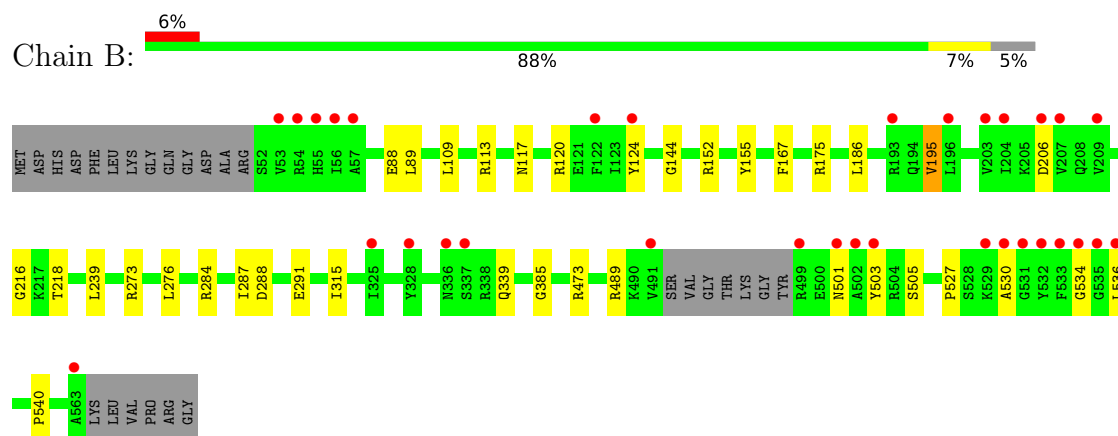
3 Residue-property plots [i](#)

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: Peptidoglycan D,D-transpeptidase FtsI



- Molecule 1: Peptidoglycan D,D-transpeptidase FtsI



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.04Å 91.14Å 148.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.92 – 1.73 46.92 – 1.73	Depositor EDS
% Data completeness (in resolution range)	74.2 (46.92-1.73) 74.2 (46.92-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.73Å)	Xtriage
Refinement program	PHENIX 1.19.1	Depositor
R, R_{free}	0.173 , 0.215 0.174 , 0.216	Depositor DCC
R_{free} test set	4266 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8813	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: CL, GOL, VL5

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	0/4067	0.49	0/5523
1	B	0.27	0/3939	0.46	0/5362
All	All	0.30	0/8006	0.48	0/10885

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

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	3962	0	3989	41	0
1	B	3841	0	3796	27	0
2	A	90	0	0	0	0
2	B	90	0	0	2	0
3	A	2	0	0	0	0
4	A	54	0	72	7	0
4	B	24	0	32	3	0
5	A	419	0	0	5	0
5	B	331	0	0	2	1
All	All	8813	0	7889	68	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 (68) 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:311[B]:LYS:NZ	5:A:701:HOH:O	2.11	0.82
1:A:327:ARG:NH1	5:A:702:HOH:O	2.16	0.78
1:B:473:ARG:HE	1:B:540:PRO:HG3	1.53	0.73
1:B:505:SER:OG	1:B:534:GLY:HA2	1.92	0.70
1:A:273:ARG:HG2	1:A:276:LEU:HD22	1.75	0.68
1:A:198:ASP:HB3	1:A:200:ARG:H	1.60	0.65
1:A:189:VAL:HB	1:A:214:LYS:HB3	1.80	0.64
1:A:381:LEU:HD22	1:A:436:MET:HG3	1.80	0.63
1:A:335:ARG:H	4:A:610:GOL:HO2	1.47	0.62
1:B:536:LEU:O	5:B:701:HOH:O	2.16	0.61
1:A:286:MET:HG2	1:A:416:ILE:HG13	1.81	0.61
1:A:394:HIS:ND1	4:A:606:GOL:H12	2.17	0.60
1:A:408:GLY:HA2	1:A:411:LEU:HD21	1.82	0.60
1:A:94:GLU:OE1	5:A:703:HOH:O	2.17	0.59
1:B:195:VAL:HA	1:B:206:ASP:HA	1.86	0.58
1:A:327:ARG:H	1:A:327:ARG:HE	1.53	0.56
1:A:505:SER:OG	1:A:534:GLY:HA2	2.06	0.56
1:B:284:ARG:HB3	4:B:602:GOL:H32	1.87	0.56
1:A:68:ARG:O	1:A:438[B]:ARG:NH1	2.38	0.54
1:A:566:VAL:HA	1:A:567:PRO:C	2.33	0.54
1:A:269:ASN:H	4:A:607:GOL:H32	1.72	0.53
1:B:152[B]:ARG:NH1	5:B:702:HOH:O	2.20	0.53
1:B:505:SER:HG	1:B:534:GLY:HA2	1.73	0.53
1:A:567:PRO:HA	1:B:113[B]:ARG:HH21	1.75	0.51
1:A:411:LEU:HD23	1:A:411:LEU:H	1.77	0.50
1:B:88:GLU:HB2	1:B:144:GLY:HA3	1.95	0.48
1:A:327:ARG:H	1:A:327:ARG:NE	2.11	0.48
1:A:547:ALA:O	1:A:551[A]:ARG:HG3	2.12	0.48
1:B:489[B]:ARG:O	2:B:601[B]:VL5:N28	2.47	0.48
1:A:298:PRO:HG3	1:A:461:LEU:HD21	1.96	0.47
1:A:503[B]:TYR:CZ	1:A:527:PRO:HG2	2.49	0.47
1:A:81:THR:OG1	1:A:150:GLU:OE2	2.20	0.46
1:B:273:ARG:O	1:B:276:LEU:HG	2.15	0.46
1:B:175:ARG:HA	1:B:175:ARG:HD3	1.73	0.46
1:B:489[B]:ARG:NH1	1:B:501:ASN:HA	2.31	0.46
1:A:438[A]:ARG:HD2	1:A:440:ASP:OD1	2.15	0.45
1:A:88:GLU:CD	1:A:202:ARG:HD3	2.42	0.44
1:A:273:ARG:HG2	1:A:276:LEU:CD2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ASN:HB3	1:B:120:ARG:HD2	1.99	0.44
1:B:218:THR:H	4:B:603:GOL:H2	1.83	0.44
1:B:291:GLU:OE1	2:B:601[A]:VL5:N28	2.50	0.44
1:A:198:ASP:OD2	1:A:202:ARG:HB3	2.18	0.44
1:A:79:VAL:HG21	1:A:152[A]:ARG:HG2	2.00	0.44
4:A:612:GOL:H11	5:A:702:HOH:O	2.16	0.44
1:A:138:ILE:HD11	1:A:147:SER:HB3	2.00	0.43
1:A:551[B]:ARG:NH2	5:A:729:HOH:O	2.50	0.43
1:A:552:LEU:HG	4:A:605:GOL:H11	2.00	0.43
1:B:288:ASP:HB2	4:B:602:GOL:H31	2.00	0.43
1:B:195:VAL:HG12	1:B:206:ASP:HB3	2.01	0.42
1:B:113[B]:ARG:NH1	1:B:124:TYR:O	2.48	0.42
1:A:51:ARG:HD3	1:A:196:LEU:HD21	2.02	0.42
1:A:305:LEU:HD22	4:A:611:GOL:H2	2.01	0.42
1:B:527:PRO:HB2	1:B:530:ALA:HB3	2.02	0.42
1:B:186:LEU:O	1:B:216:GLY:HA3	2.20	0.41
1:B:287:ILE:HG12	1:B:385:GLY:O	2.20	0.41
1:B:155:TYR:OH	1:B:167:PHE:HA	2.20	0.41
1:B:315:ILE:CG2	1:B:339:GLN:HB3	2.50	0.41
1:A:291[B]:GLU:CD	1:A:410:GLY:H	2.27	0.41
1:A:316:VAL:HB	1:A:345:ILE:HD11	2.03	0.41
1:A:551[A]:ARG:HD2	4:A:605:GOL:O2	2.20	0.41
1:B:109:LEU:HD23	1:B:109:LEU:HA	1.90	0.41
1:A:181:ALA:HB2	1:A:384:PRO:HD3	2.01	0.41
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.91	0.41
1:A:127:ARG:NH1	1:A:152[A]:ARG:HH22	2.19	0.41
1:A:536[B]:LEU:HD12	1:A:537:VAL:HG23	2.03	0.41
1:A:438[A]:ARG:NH1	1:A:440:ASP:OD2	2.55	0.40
1:B:503[B]:TYR:CZ	1:B:527:PRO:HG2	2.57	0.40
1:A:276:LEU:HD21	1:A:281:MET:HG2	2.03	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)
5:B:961:HOH:O	5:B:969:HOH:O[3_455]	2.07	0.13

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	522/531 (98%)	510 (98%)	12 (2%)	0	100	100
1	B	514/531 (97%)	503 (98%)	11 (2%)	0	100	100
All	All	1036/1062 (98%)	1013 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	407/423 (96%)	405 (100%)	2 (0%)	81	75
1	B	390/423 (92%)	388 (100%)	2 (0%)	81	75
All	All	797/846 (94%)	793 (100%)	4 (0%)	81	75

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	LEU
1	A	327	ARG
1	B	195	VAL
1	B	239	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	85	ASN
1	A	351	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	$\# Z > 2$
4	GOL	B	602	-	5,5,5	0.11	0	5,5,5	0.26	0
2	VL5	B	601[B]	1	41,47,47	1.62	4 (9%)	41,66,66	2.00	8 (19%)
4	GOL	A	609	-	5,5,5	0.11	0	5,5,5	0.36	0
4	GOL	A	604	-	5,5,5	0.11	0	5,5,5	0.12	0
2	VL5	B	601[A]	1	41,47,47	1.61	4 (9%)	41,66,66	1.77	7 (17%)
4	GOL	A	607	-	5,5,5	0.08	0	5,5,5	0.29	0
4	GOL	A	611	-	5,5,5	0.12	0	5,5,5	0.33	0
4	GOL	A	606	-	5,5,5	0.08	0	5,5,5	0.21	0
2	VL5	A	601[B]	1	41,47,47	1.61	5 (12%)	41,66,66	1.81	5 (12%)
4	GOL	A	608	-	5,5,5	0.08	0	5,5,5	0.26	0
4	GOL	B	604	-	5,5,5	0.11	0	5,5,5	0.38	0
4	GOL	B	605	-	5,5,5	0.11	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	610	-	5,5,5	0.10	0	5,5,5	0.31	0
4	GOL	A	612	-	5,5,5	0.20	0	5,5,5	0.24	0
2	VL5	A	601[A]	1	41,47,47	1.56	4 (9%)	41,66,66	1.90	8 (19%)
4	GOL	A	605	-	5,5,5	0.11	0	5,5,5	0.40	0
4	GOL	B	603	-	5,5,5	0.08	0	5,5,5	0.30	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
4	GOL	B	602	-	-	0/4/4/4	-
2	VL5	B	601[B]	1	-	7/38/57/57	0/3/3/3
4	GOL	A	609	-	-	0/4/4/4	-
4	GOL	A	604	-	-	0/4/4/4	-
2	VL5	B	601[A]	1	-	9/38/57/57	0/3/3/3
4	GOL	A	607	-	-	0/4/4/4	-
4	GOL	A	611	-	-	0/4/4/4	-
4	GOL	A	606	-	-	0/4/4/4	-
2	VL5	A	601[B]	1	-	12/38/57/57	0/3/3/3
4	GOL	A	608	-	-	1/4/4/4	-
4	GOL	B	604	-	-	0/4/4/4	-
4	GOL	B	605	-	-	0/4/4/4	-
4	GOL	A	610	-	-	0/4/4/4	-
4	GOL	A	612	-	-	0/4/4/4	-
2	VL5	A	601[A]	1	-	11/38/57/57	0/3/3/3
4	GOL	A	605	-	-	0/4/4/4	-
4	GOL	B	603	-	-	0/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601[B]	VL5	O22-N23	-6.46	1.26	1.41
2	A	601[A]	VL5	O22-N23	-6.39	1.26	1.41
2	B	601[B]	VL5	O22-N23	-6.28	1.26	1.41
2	B	601[A]	VL5	O22-N23	-6.12	1.27	1.41
2	B	601[A]	VL5	C27-N28	5.80	1.45	1.34
2	B	601[B]	VL5	C27-N28	5.70	1.45	1.34
2	A	601[B]	VL5	C27-N28	5.11	1.44	1.34
2	A	601[A]	VL5	C27-N28	4.82	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601[A]	VL5	C30-C25	2.79	1.41	1.36
2	B	601[B]	VL5	C30-C25	2.78	1.41	1.36
2	A	601[B]	VL5	C30-C25	2.73	1.41	1.36
2	A	601[A]	VL5	C30-C25	2.69	1.41	1.36
2	B	601[A]	VL5	C27-N26	2.36	1.35	1.31
2	B	601[B]	VL5	C27-N26	2.22	1.34	1.31
2	A	601[B]	VL5	C18-C19	-2.10	1.49	1.52
2	A	601[B]	VL5	C27-S29	-2.03	1.71	1.74
2	A	601[A]	VL5	C27-S29	-2.00	1.71	1.74

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601[A]	VL5	O22-N23-C24	8.18	121.02	111.72
2	B	601[B]	VL5	O22-N23-C24	7.85	120.64	111.72
2	B	601[A]	VL5	O22-N23-C24	7.15	119.84	111.72
2	A	601[B]	VL5	O22-N23-C24	7.04	119.72	111.72
2	B	601[B]	VL5	C30-S29-C27	5.99	91.42	88.84
2	B	601[A]	VL5	C30-S29-C27	5.30	91.13	88.84
2	A	601[B]	VL5	C30-S29-C27	4.96	90.98	88.84
2	A	601[A]	VL5	C30-S29-C27	4.26	90.68	88.84
2	B	601[B]	VL5	C3-N7-C8	3.91	128.43	122.75
2	A	601[B]	VL5	C10-C8-N7	3.89	120.52	114.60
2	A	601[A]	VL5	C10-C8-N7	3.77	120.33	114.60
2	B	601[B]	VL5	S29-C27-N28	2.83	124.29	120.99
2	A	601[A]	VL5	C24-C31-N33	2.83	118.74	114.27
2	A	601[B]	VL5	C24-C31-N33	2.80	118.69	114.27
2	A	601[A]	VL5	S29-C27-N28	2.79	124.23	120.99
2	B	601[A]	VL5	C10-C8-N7	2.78	118.83	114.60
2	B	601[A]	VL5	S29-C27-N28	2.52	123.92	120.99
2	A	601[B]	VL5	S29-C27-N28	2.36	123.74	120.99
2	B	601[A]	VL5	C24-C31-N33	2.30	117.89	114.27
2	B	601[B]	VL5	O20-C19-C18	2.23	118.52	112.71
2	A	601[A]	VL5	O20-C19-C18	2.21	118.45	112.71
2	A	601[A]	VL5	N28-C27-N26	-2.14	121.56	124.05
2	B	601[B]	VL5	O21-C19-C18	-2.14	118.23	122.85
2	B	601[A]	VL5	O21-C19-C18	-2.09	118.33	122.85
2	A	601[A]	VL5	O21-C19-C18	-2.07	118.38	122.85
2	B	601[B]	VL5	C24-C31-N33	2.07	117.53	114.27
2	B	601[A]	VL5	O20-C19-C18	2.04	118.02	112.71
2	B	601[B]	VL5	C10-C8-N7	2.03	117.69	114.60

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601[A]	VL5	C4-C3-N7-C8
2	A	601[A]	VL5	C39-C34-C35-C36
2	A	601[A]	VL5	C39-C34-C35-C37
2	A	601[A]	VL5	N33-C34-C35-C36
2	A	601[A]	VL5	N33-C34-C35-C37
2	A	601[A]	VL5	C10-C8-N7-C3
2	A	601[A]	VL5	N9-C8-N7-C3
2	A	601[B]	VL5	O16-C17-C18-C19
2	A	601[B]	VL5	O16-C17-C18-O22
2	A	601[B]	VL5	C39-C34-C35-C36
2	A	601[B]	VL5	C39-C34-C35-C37
2	A	601[B]	VL5	N33-C34-C35-C36
2	A	601[B]	VL5	N33-C34-C35-C37
2	B	601[A]	VL5	O16-C17-C18-O22
2	B	601[A]	VL5	C39-C34-C35-C36
2	B	601[A]	VL5	C39-C34-C35-C37
2	B	601[A]	VL5	N33-C34-C35-C36
2	B	601[A]	VL5	N33-C34-C35-C37
2	B	601[B]	VL5	C39-C34-C35-C36
2	B	601[B]	VL5	C39-C34-C35-C37
2	B	601[B]	VL5	N33-C34-C35-C36
2	B	601[B]	VL5	N33-C34-C35-C37
2	A	601[B]	VL5	C12-C13-O16-C17
2	A	601[B]	VL5	C14-C13-O16-C17
2	B	601[A]	VL5	O16-C17-C18-C19
2	A	601[A]	VL5	C15-C10-C8-N7
2	A	601[B]	VL5	C11-C10-C8-N7
2	A	601[B]	VL5	C15-C10-C8-N7
4	A	608	GOL	O1-C1-C2-C3
2	A	601[A]	VL5	C11-C10-C8-N7
2	A	601[A]	VL5	N23-C24-C31-O32
2	A	601[B]	VL5	N23-C24-C31-O32
2	A	601[A]	VL5	N23-C24-C31-N33
2	A	601[B]	VL5	N23-C24-C31-N33
2	B	601[A]	VL5	N23-C24-C31-N33
2	B	601[B]	VL5	C4-C3-N7-C8
2	B	601[A]	VL5	C15-C10-C8-N9
2	B	601[B]	VL5	N23-C24-C31-N33
2	B	601[A]	VL5	N23-C24-C31-O32
2	B	601[B]	VL5	N23-C24-C31-O32

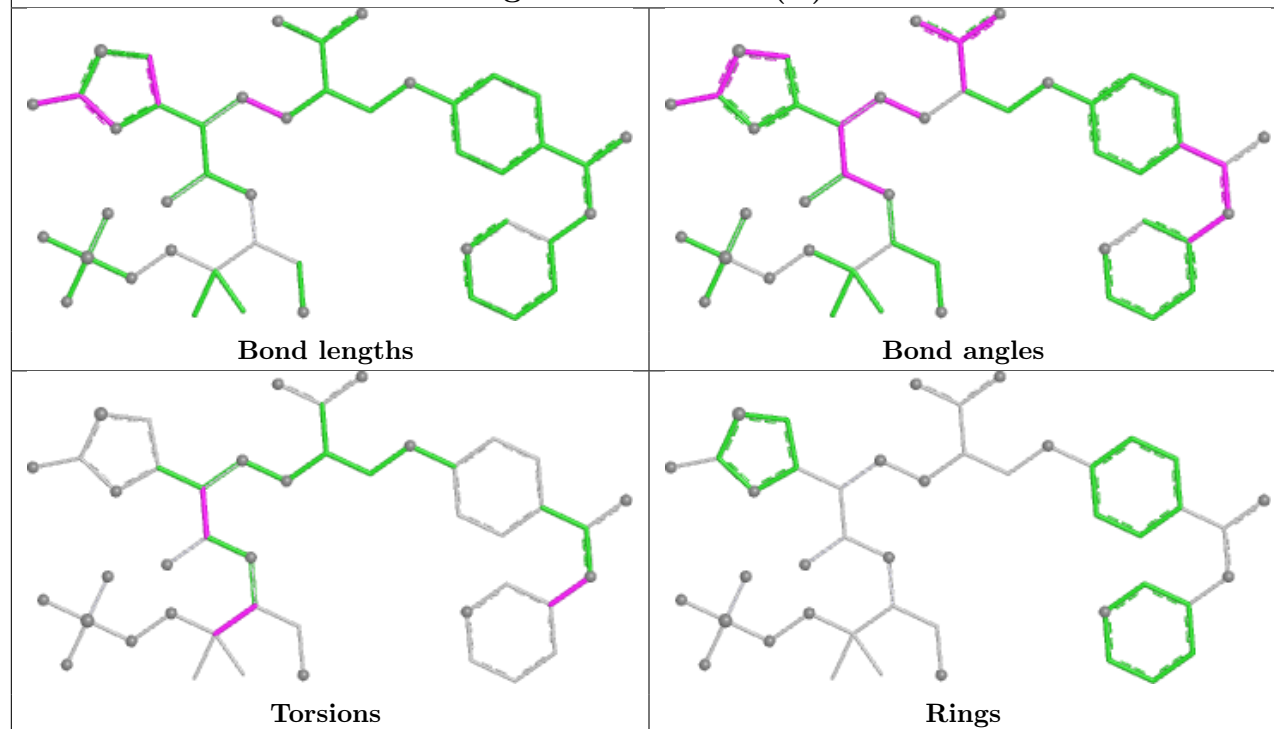
There are no ring outliers.

10 monomers are involved in 12 short contacts:

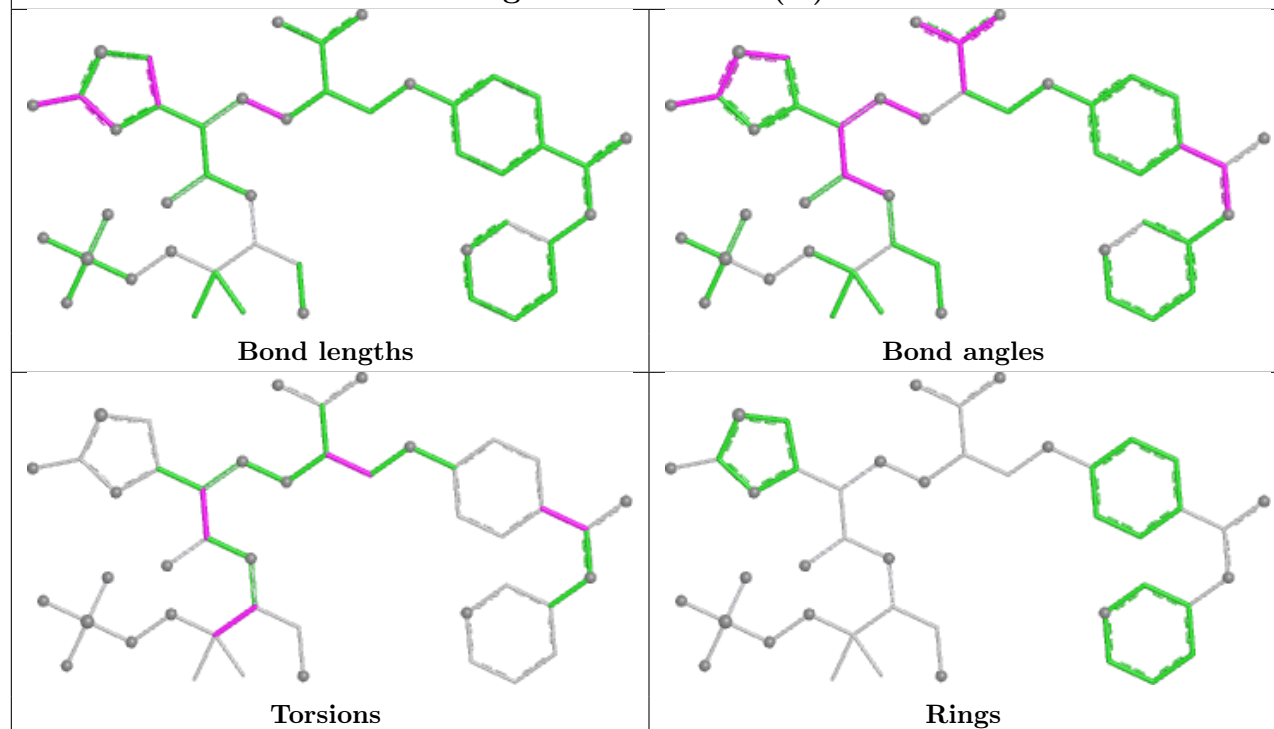
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	GOL	2	0
2	B	601[B]	VL5	1	0
2	B	601[A]	VL5	1	0
4	A	607	GOL	1	0
4	A	611	GOL	1	0
4	A	606	GOL	1	0
4	A	610	GOL	1	0
4	A	612	GOL	1	0
4	A	605	GOL	2	0
4	B	603	GOL	1	0

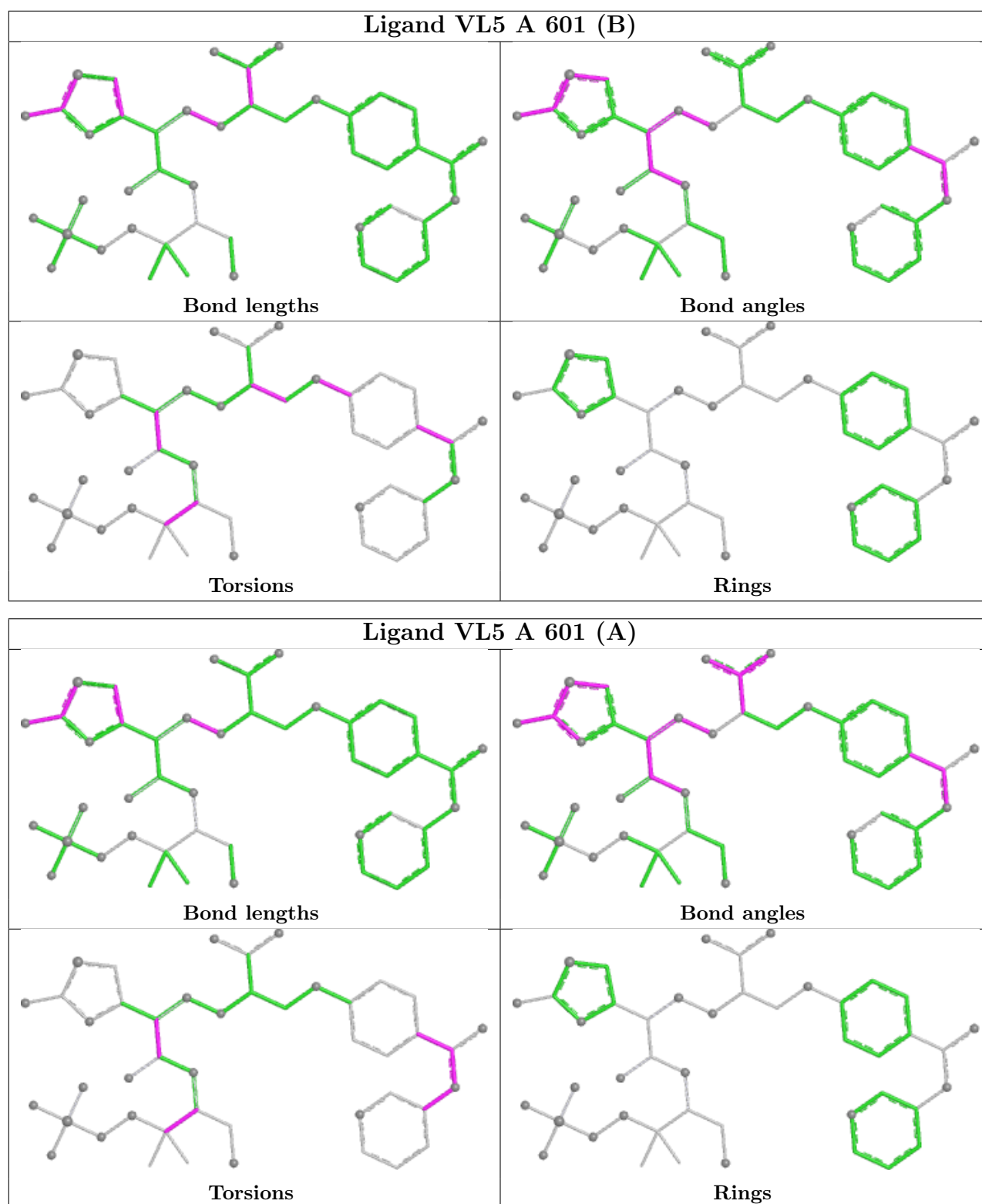
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand VL5 B 601 (B)



Ligand VL5 B 601 (A)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	512/531 (96%)	0.23	45 (8%) 15 20	10, 24, 77, 136	18 (3%)
1	B	505/531 (95%)	0.22	32 (6%) 26 32	12, 28, 68, 101	16 (3%)
All	All	1017/1062 (95%)	0.22	77 (7%) 20 25	10, 26, 74, 136	34 (3%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	533[A]	PHE	9.5
1	A	536[A]	LEU	8.8
1	A	533[A]	PHE	8.5
1	A	532[A]	TYR	7.4
1	A	207	VAL	6.8
1	B	531[A]	GLY	6.7
1	B	532[A]	TYR	5.8
1	B	536	LEU	5.2
1	B	535	GLY	4.9
1	B	534	GLY	4.8
1	A	565	LEU	4.6
1	A	566	VAL	4.3
1	A	567	PRO	4.3
1	A	534	GLY	4.2
1	B	53	VAL	4.2
1	A	50	ALA	4.1
1	B	499	ARG	4.0
1	A	529	LYS	3.9
1	A	492	SER	3.9
1	A	83	TRP	3.9
1	B	55	HIS	3.8
1	A	493	VAL	3.8
1	A	209	VAL	3.7
1	A	210	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	56	ILE	3.6
1	A	535	GLY	3.5
1	A	146	TYR	3.4
1	B	503[A]	TYR	3.4
1	B	204	ILE	3.4
1	B	328	TYR	3.3
1	A	204	ILE	3.3
1	B	207	VAL	3.3
1	B	336	ASN	3.3
1	A	195	VAL	3.2
1	B	529	LYS	3.2
1	B	491	VAL	3.2
1	A	203	VAL	3.2
1	B	337[A]	SER	3.1
1	A	201	GLY	3.1
1	A	152[A]	ARG	3.1
1	A	501	ASN	3.0
1	A	124	TYR	3.0
1	A	211	LYS	3.0
1	A	53	VAL	2.9
1	B	530	ALA	2.9
1	B	54	ARG	2.8
1	A	500	GLU	2.8
1	A	205	LYS	2.8
1	A	196	LEU	2.7
1	B	501	ASN	2.7
1	A	200	ARG	2.7
1	B	563	ALA	2.7
1	B	325	ILE	2.6
1	A	491	VAL	2.5
1	A	122	PHE	2.5
1	B	206	ASP	2.5
1	A	48	GLY	2.5
1	A	49	ASP	2.5
1	A	199	ARG	2.4
1	A	59	PRO	2.3
1	A	206	ASP	2.3
1	B	57	ALA	2.3
1	B	196	LEU	2.3
1	A	324	GLN	2.3
1	B	124	TYR	2.3
1	A	148	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	145	VAL	2.3
1	B	122	PHE	2.2
1	A	138	ILE	2.2
1	A	208	GLN	2.2
1	A	198	ASP	2.1
1	A	56	ILE	2.1
1	B	193	ARG	2.1
1	B	209	VAL	2.0
1	A	212	ASN	2.0
1	B	502	ALA	2.0
1	B	203	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	603	6/6	0.70	0.13	48,54,57,57	0
4	GOL	B	604	6/6	0.76	0.14	46,49,55,55	0
4	GOL	A	609	6/6	0.79	0.16	41,46,53,55	0
4	GOL	A	611	6/6	0.80	0.12	28,37,41,44	0
4	GOL	B	605	6/6	0.83	0.11	38,44,49,53	0
4	GOL	A	607	6/6	0.84	0.12	34,41,51,56	0
4	GOL	A	605	6/6	0.84	0.13	38,41,44,47	0
4	GOL	A	610	6/6	0.85	0.12	30,44,49,50	0
4	GOL	A	604	6/6	0.86	0.14	25,27,29,44	0
2	VL5	A	601[B]	45/45	0.87	0.18	16,38,53,57	45
4	GOL	A	606	6/6	0.87	0.11	31,40,44,51	0
2	VL5	A	601[A]	45/45	0.87	0.18	16,38,61,63	45

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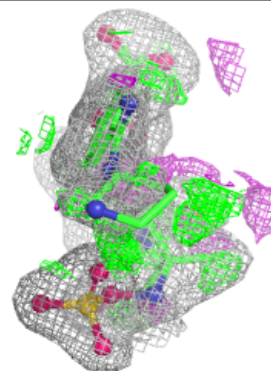
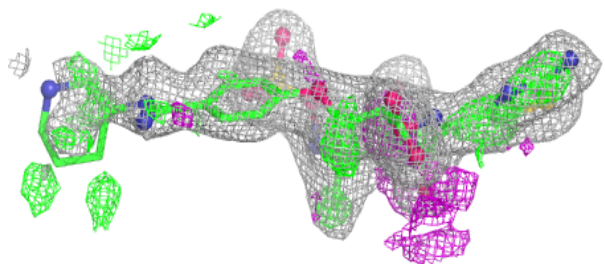
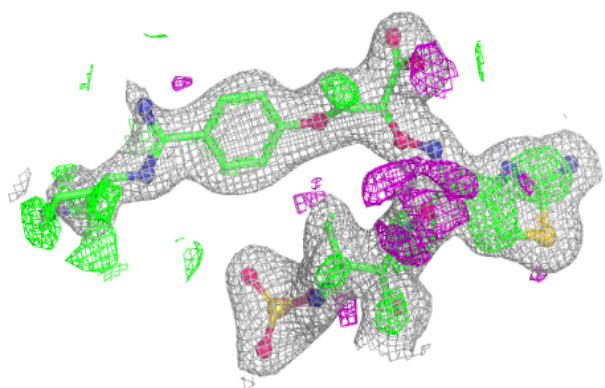
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	608	6/6	0.89	0.11	27,28,41,43	0
3	CL	A	603	1/1	0.90	0.17	54,54,54,54	0
2	VL5	B	601[B]	45/45	0.92	0.10	20,29,35,37	45
2	VL5	B	601[A]	45/45	0.92	0.10	20,29,36,38	45
4	GOL	A	612	6/6	0.92	0.19	14,30,46,47	0
4	GOL	B	602	6/6	0.93	0.11	18,29,38,40	0
3	CL	A	602	1/1	0.94	0.17	44,44,44,44	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.

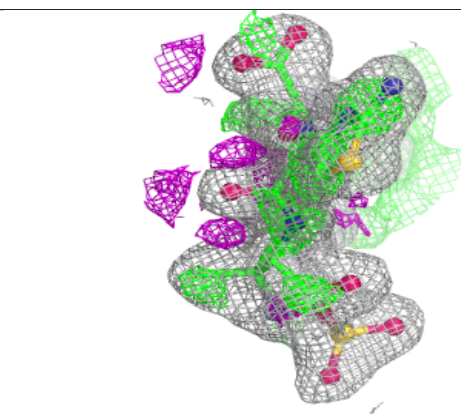
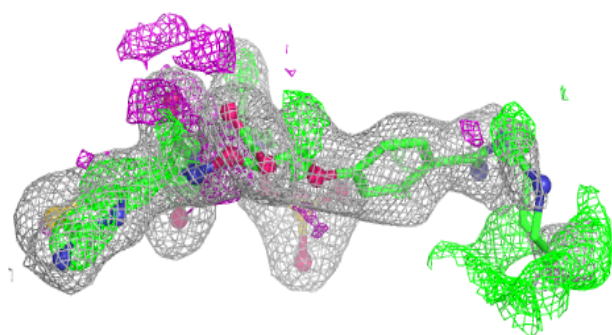
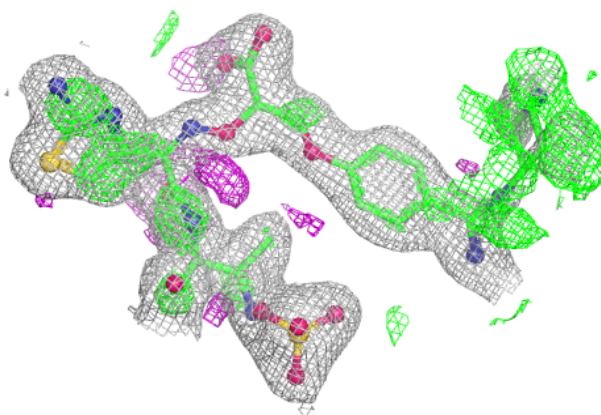
Electron density around VL5 A 601 (B):

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

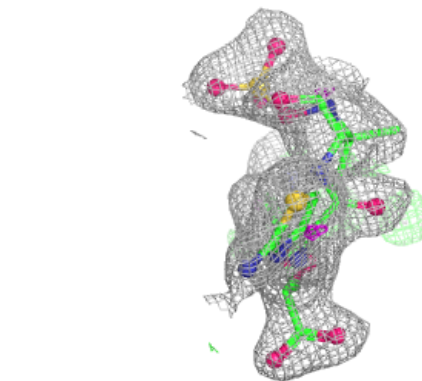
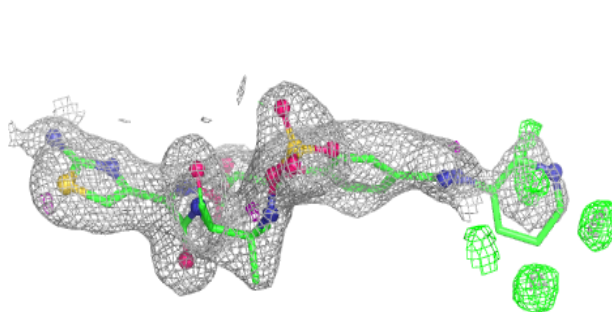
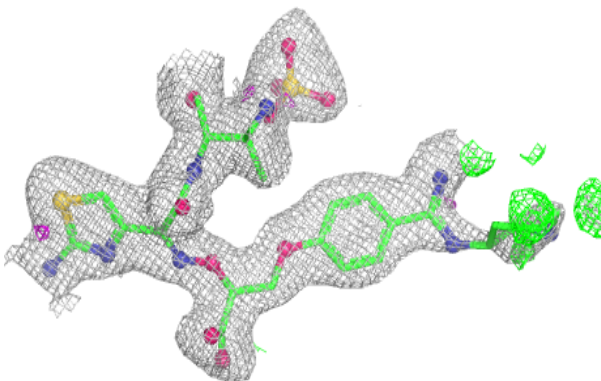


Electron density around VL5 A 601 (A):

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

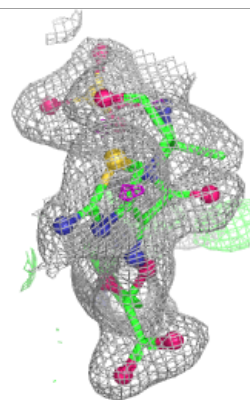
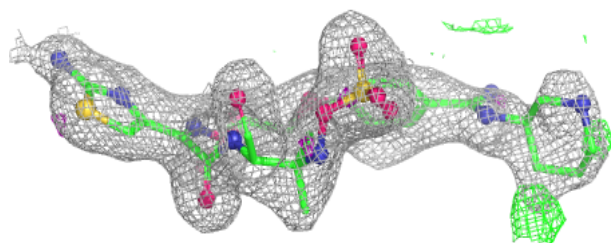
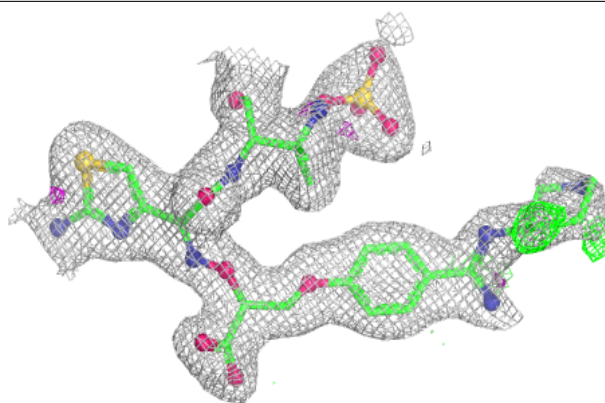
**Electron density around VL5 B 601 (B):**

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



Electron density around VL5 B 601 (A):

$2mF_o-DF_c$ (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.