



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:39 AM UTC

PDB ID : 8OMD / pdb_00008omd
Title : Crystal structure of mKHK in complex with compound-4
Authors : Ebenhoch, R.; Pautsch, A.
Deposited on : 2023-03-31
Resolution : 2.00 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

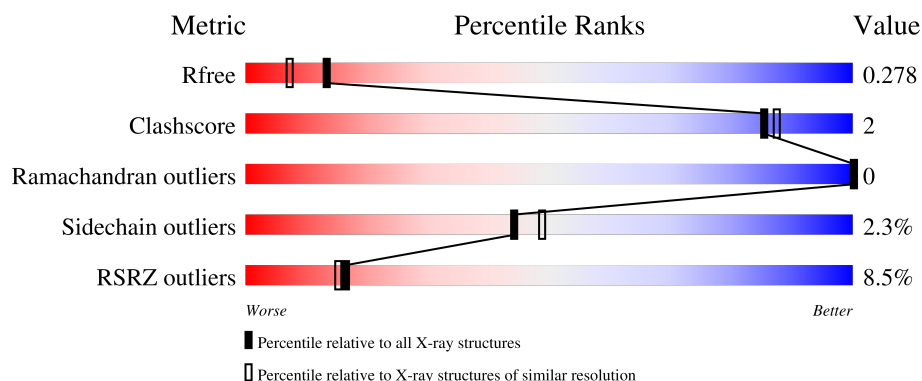
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	316	4% 86% 7% • 6%
1	B	316	5% 88% 5% • 6%
1	C	316	8% 84% 9% • 6%
1	D	316	14% 86% 6% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9534 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 Ketohexokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2280	1430	405	432	13			
1	B	296	Total	C	N	O	S	0	0	0
			2280	1430	405	432	13			
1	C	296	Total	C	N	O	S	0	0	0
			2280	1430	405	432	13			
1	D	295	Total	C	N	O	S	0	0	0
			2271	1425	404	429	13			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP A0A0J9YU79
A	-16	GLY	-	expression tag	UNP A0A0J9YU79
A	-15	SER	-	expression tag	UNP A0A0J9YU79
A	-14	SER	-	expression tag	UNP A0A0J9YU79
A	-13	HIS	-	expression tag	UNP A0A0J9YU79
A	-12	HIS	-	expression tag	UNP A0A0J9YU79
A	-11	HIS	-	expression tag	UNP A0A0J9YU79
A	-10	HIS	-	expression tag	UNP A0A0J9YU79
A	-9	HIS	-	expression tag	UNP A0A0J9YU79
A	-8	HIS	-	expression tag	UNP A0A0J9YU79
A	-7	SER	-	expression tag	UNP A0A0J9YU79
A	-6	SER	-	expression tag	UNP A0A0J9YU79
A	-5	GLY	-	expression tag	UNP A0A0J9YU79
A	-4	LEU	-	expression tag	UNP A0A0J9YU79
A	-3	VAL	-	expression tag	UNP A0A0J9YU79
A	-2	PRO	-	expression tag	UNP A0A0J9YU79
A	-1	ARG	-	expression tag	UNP A0A0J9YU79
A	0	GLY	-	expression tag	UNP A0A0J9YU79
A	1	GLY	-	expression tag	UNP A0A0J9YU79
B	-17	MET	-	initiating methionine	UNP A0A0J9YU79
B	-16	GLY	-	expression tag	UNP A0A0J9YU79

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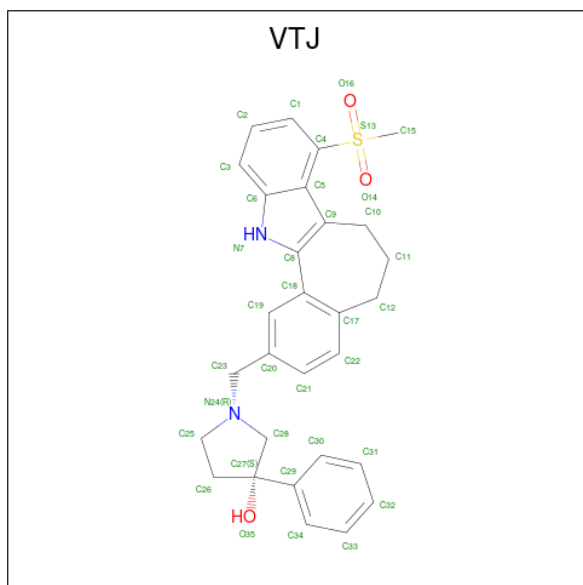
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	SER	-	expression tag	UNP A0A0J9YU79
B	-14	SER	-	expression tag	UNP A0A0J9YU79
B	-13	HIS	-	expression tag	UNP A0A0J9YU79
B	-12	HIS	-	expression tag	UNP A0A0J9YU79
B	-11	HIS	-	expression tag	UNP A0A0J9YU79
B	-10	HIS	-	expression tag	UNP A0A0J9YU79
B	-9	HIS	-	expression tag	UNP A0A0J9YU79
B	-8	HIS	-	expression tag	UNP A0A0J9YU79
B	-7	SER	-	expression tag	UNP A0A0J9YU79
B	-6	SER	-	expression tag	UNP A0A0J9YU79
B	-5	GLY	-	expression tag	UNP A0A0J9YU79
B	-4	LEU	-	expression tag	UNP A0A0J9YU79
B	-3	VAL	-	expression tag	UNP A0A0J9YU79
B	-2	PRO	-	expression tag	UNP A0A0J9YU79
B	-1	ARG	-	expression tag	UNP A0A0J9YU79
B	0	GLY	-	expression tag	UNP A0A0J9YU79
B	1	GLY	-	expression tag	UNP A0A0J9YU79
C	-17	MET	-	initiating methionine	UNP A0A0J9YU79
C	-16	GLY	-	expression tag	UNP A0A0J9YU79
C	-15	SER	-	expression tag	UNP A0A0J9YU79
C	-14	SER	-	expression tag	UNP A0A0J9YU79
C	-13	HIS	-	expression tag	UNP A0A0J9YU79
C	-12	HIS	-	expression tag	UNP A0A0J9YU79
C	-11	HIS	-	expression tag	UNP A0A0J9YU79
C	-10	HIS	-	expression tag	UNP A0A0J9YU79
C	-9	HIS	-	expression tag	UNP A0A0J9YU79
C	-8	HIS	-	expression tag	UNP A0A0J9YU79
C	-7	SER	-	expression tag	UNP A0A0J9YU79
C	-6	SER	-	expression tag	UNP A0A0J9YU79
C	-5	GLY	-	expression tag	UNP A0A0J9YU79
C	-4	LEU	-	expression tag	UNP A0A0J9YU79
C	-3	VAL	-	expression tag	UNP A0A0J9YU79
C	-2	PRO	-	expression tag	UNP A0A0J9YU79
C	-1	ARG	-	expression tag	UNP A0A0J9YU79
C	0	GLY	-	expression tag	UNP A0A0J9YU79
C	1	GLY	-	expression tag	UNP A0A0J9YU79
D	-17	MET	-	initiating methionine	UNP A0A0J9YU79
D	-16	GLY	-	expression tag	UNP A0A0J9YU79
D	-15	SER	-	expression tag	UNP A0A0J9YU79
D	-14	SER	-	expression tag	UNP A0A0J9YU79
D	-13	HIS	-	expression tag	UNP A0A0J9YU79
D	-12	HIS	-	expression tag	UNP A0A0J9YU79

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	HIS	-	expression tag	UNP A0A0J9YU79
D	-10	HIS	-	expression tag	UNP A0A0J9YU79
D	-9	HIS	-	expression tag	UNP A0A0J9YU79
D	-8	HIS	-	expression tag	UNP A0A0J9YU79
D	-7	SER	-	expression tag	UNP A0A0J9YU79
D	-6	SER	-	expression tag	UNP A0A0J9YU79
D	-5	GLY	-	expression tag	UNP A0A0J9YU79
D	-4	LEU	-	expression tag	UNP A0A0J9YU79
D	-3	VAL	-	expression tag	UNP A0A0J9YU79
D	-2	PRO	-	expression tag	UNP A0A0J9YU79
D	-1	ARG	-	expression tag	UNP A0A0J9YU79
D	0	GLY	-	expression tag	UNP A0A0J9YU79
D	1	GLY	-	expression tag	UNP A0A0J9YU79

- Molecule 2 is compound (CCD ID: VTJ) (formula: $C_{29}H_{30}N_2O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	29	2	3	1		
2	B	1	Total	C	N	O	S	0	0
			35	29	2	3	1		
2	C	1	Total	C	N	O	S	0	0
			35	29	2	3	1		
2	D	1	Total	C	N	O	S	0	0
			35	29	2	3	1		

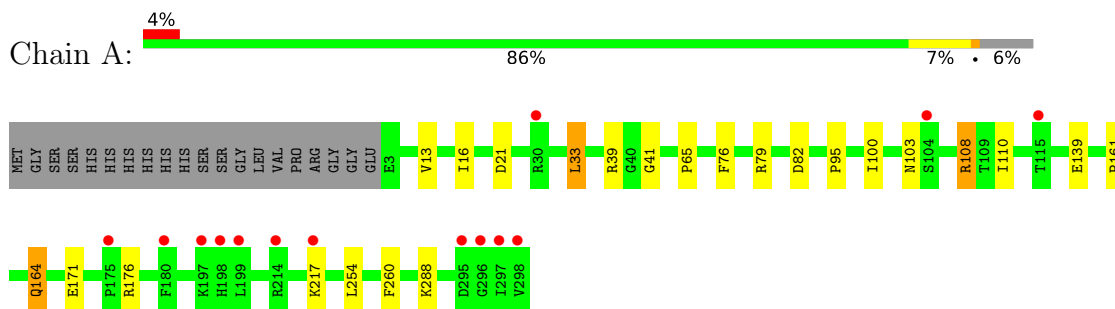
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	84	Total 84	O 84	0	0
3	B	88	Total 88	O 88	0	0
3	C	54	Total 54	O 54	0	0
3	D	57	Total 57	O 57	0	0

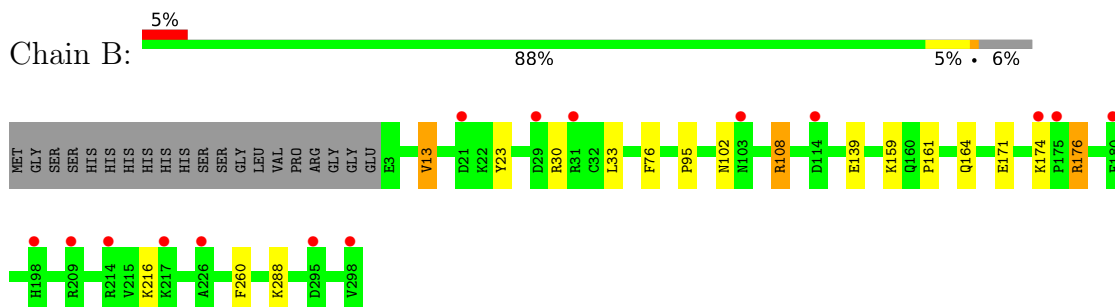
3 Residue-property plots [i](#)

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.

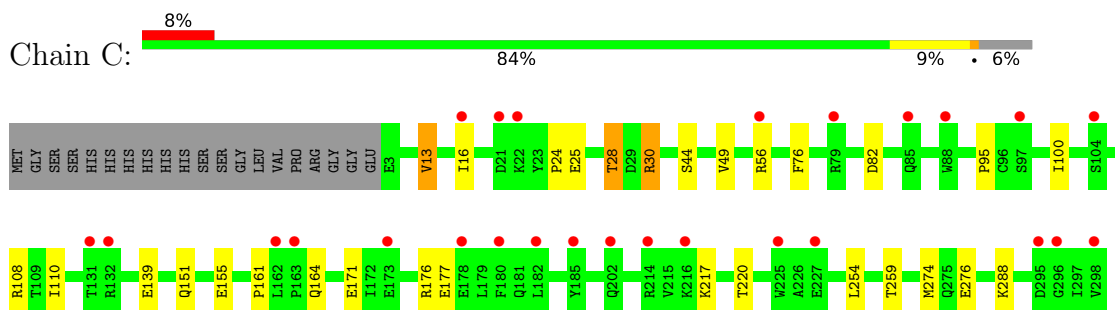
- Molecule 1: Ketohexokinase



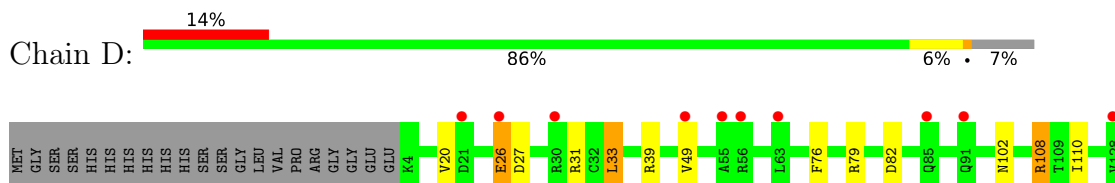
- Molecule 1: Ketohexokinase

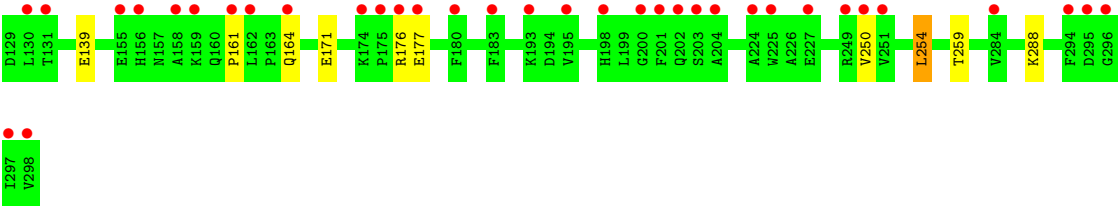


- Molecule 1: Ketohexokinase



- Molecule 1: Ketohexokinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.42Å 55.60Å 136.63Å 91.40° 93.10° 115.34°	Depositor
Resolution (Å)	47.92 – 2.00 47.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (47.92-2.00) 95.7 (47.92-2.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.00Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.235 , 0.266 0.249 , 0.278	Depositor DCC
R_{free} test set	4085 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9534	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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: VTJ

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	0.80	0/2321	1.26	7/3138 (0.2%)
1	B	0.79	0/2321	1.26	6/3138 (0.2%)
1	C	0.78	0/2321	1.25	5/3138 (0.2%)
1	D	0.79	0/2312	1.27	8/3126 (0.3%)
All	All	0.79	0/9275	1.26	26/12540 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ASN	CA-CB-CG	6.78	119.38	112.60
1	D	26	GLU	CB-CG-CD	6.07	122.91	112.60
1	D	33	LEU	N-CA-C	-5.76	104.60	111.69
1	A	82	ASP	CA-CB-CG	5.59	118.19	112.60
1	C	276	GLU	CB-CG-CD	5.46	121.89	112.60
1	D	76	PHE	CA-CB-CG	5.43	119.23	113.80
1	D	82	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	176	ARG	CA-C-N	5.42	127.86	120.54
1	A	176	ARG	C-N-CA	5.42	127.86	120.54
1	B	76	PHE	CA-CB-CG	5.36	119.16	113.80
1	A	76	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	33	LEU	N-CA-C	-5.31	105.16	111.69
1	D	176	ARG	CA-C-N	5.28	127.67	120.54
1	D	176	ARG	C-N-CA	5.28	127.67	120.54
1	B	176	ARG	CA-C-N	5.26	127.59	120.38
1	B	176	ARG	C-N-CA	5.26	127.59	120.38
1	A	41	GLY	N-CA-C	-5.25	106.12	112.48
1	C	82	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	33	LEU	N-CA-C	-5.20	105.30	111.69
1	D	102	ASN	CA-C-N	5.19	127.75	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	102	ASN	C-N-CA	5.19	127.75	120.28
1	C	76	PHE	CA-CB-CG	5.10	118.90	113.80
1	C	176	ARG	CA-C-N	5.09	127.41	120.54
1	C	176	ARG	C-N-CA	5.09	127.41	120.54
1	B	102	ASN	CA-C-N	5.00	127.48	120.28
1	B	102	ASN	C-N-CA	5.00	127.48	120.28

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	2280	0	2263	11	0
1	B	2280	0	2263	13	0
1	C	2280	0	2263	11	0
1	D	2271	0	2257	14	0
2	A	35	0	0	1	0
2	B	35	0	0	1	0
2	C	35	0	0	0	0
2	D	35	0	0	0	0
3	A	84	0	0	0	0
3	B	88	0	0	0	0
3	C	54	0	0	0	0
3	D	57	0	0	0	0
All	All	9534	0	9046	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 2.

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)
1:A:65:PRO:HB3	1:B:159:LYS:HG2	1.66	0.77
1:B:23:TYR:CG	1:D:26:GLU:HG3	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:HD13	1:C:16:ILE:HD13	1.71	0.72
1:B:176:ARG:NH1	1:D:31:ARG:HH12	1.92	0.68
1:B:23:TYR:CD2	1:D:26:GLU:HG3	2.29	0.68
1:B:139:GLU:HA	1:B:171:GLU:HG2	1.78	0.66
1:B:13:VAL:HB	1:B:95:PRO:HB2	1.78	0.65
1:A:39:ARG:HH11	1:A:79:ARG:HD2	1.63	0.64
1:C:13:VAL:HB	1:C:95:PRO:HB2	1.79	0.64
1:D:39:ARG:HH11	1:D:79:ARG:HD2	1.64	0.64
1:A:139:GLU:HA	1:A:171:GLU:HG2	1.86	0.57
1:B:174:LYS:HG2	1:B:176:ARG:CZ	2.40	0.52
1:C:220:THR:HG21	1:C:274:MET:HE3	1.92	0.52
1:C:24:PRO:HB3	1:C:30:ARG:HD2	1.93	0.50
1:A:260:PHE:HB2	2:A:301:VTJ:C15	2.41	0.50
1:D:139:GLU:HA	1:D:171:GLU:HG2	1.94	0.50
1:D:161:PRO:HD2	1:D:164:GLN:HB2	1.95	0.49
1:A:161:PRO:HD2	1:A:164:GLN:HB2	1.97	0.47
1:D:39:ARG:NH1	1:D:79:ARG:HD2	2.28	0.47
1:D:108:ARG:HH21	1:D:110:ILE:HD12	1.80	0.47
1:C:161:PRO:HD2	1:C:164:GLN:HB2	1.98	0.46
1:B:260:PHE:HB2	2:B:301:VTJ:C15	2.47	0.45
1:D:49:VAL:HG21	1:D:259:THR:HA	1.98	0.45
1:A:108:ARG:O	1:A:108:ARG:HD3	2.17	0.44
1:B:161:PRO:HD2	1:B:164:GLN:HB2	2.00	0.44
1:B:176:ARG:NH1	1:D:31:ARG:NH1	2.65	0.43
1:D:110:ILE:HD11	1:D:254:LEU:HD23	1.99	0.43
1:B:108:ARG:O	1:B:108:ARG:HD3	2.19	0.43
1:B:176:ARG:CZ	1:D:31:ARG:HH12	2.31	0.43
1:B:108:ARG:O	1:D:27:ASP:HA	2.19	0.43
1:C:151:GLN:O	1:C:155:GLU:HG2	2.20	0.42
1:A:13:VAL:HG22	1:A:95:PRO:HB2	2.01	0.42
1:C:139:GLU:HA	1:C:171:GLU:HG2	2.02	0.41
1:A:100:ILE:HD11	1:C:100:ILE:HD11	2.02	0.41
1:C:25:GLU:O	1:C:28:THR:HG22	2.19	0.41
1:A:110:ILE:HD11	1:A:254:LEU:HD13	2.02	0.41
1:C:110:ILE:HD11	1:C:254:LEU:HD13	2.03	0.41
1:D:20:VAL:HA	1:D:33:LEU:HD13	2.02	0.41
1:A:21:ASP:HB3	1:A:33:LEU:HD11	2.02	0.41
1:C:49:VAL:HG21	1:C:259:THR:HA	2.02	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	294/316 (93%)	286 (97%)	8 (3%)	0	100	100
1	B	294/316 (93%)	287 (98%)	7 (2%)	0	100	100
1	C	294/316 (93%)	286 (97%)	8 (3%)	0	100	100
1	D	293/316 (93%)	286 (98%)	7 (2%)	0	100	100
All	All	1175/1264 (93%)	1145 (97%)	30 (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	249/265 (94%)	245 (98%)	4 (2%)	55	62
1	B	249/265 (94%)	244 (98%)	5 (2%)	48	54
1	C	249/265 (94%)	240 (96%)	9 (4%)	31	31
1	D	248/265 (94%)	243 (98%)	5 (2%)	48	54
All	All	995/1060 (94%)	972 (98%)	23 (2%)	44	49

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ARG
1	A	164	GLN

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Mol	Chain	Res	Type
1	A	217	LYS
1	A	288	LYS
1	B	13	VAL
1	B	30	ARG
1	B	108	ARG
1	B	216	LYS
1	B	288	LYS
1	C	13	VAL
1	C	28	THR
1	C	30	ARG
1	C	44	SER
1	C	56	ARG
1	C	108	ARG
1	C	177	GLU
1	C	217	LYS
1	C	288	LYS
1	D	108	ARG
1	D	177	GLU
1	D	250	VAL
1	D	254	LEU
1	D	288	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	35	GLN
1	A	78	GLN
1	A	164	GLN
1	A	261	ASN
1	A	275	GLN
1	A	283	GLN
1	B	78	GLN
1	B	261	ASN
1	B	283	GLN
1	C	18	ASN
1	C	35	GLN
1	C	261	ASN
1	C	275	GLN
1	C	283	GLN
1	D	18	ASN
1	D	35	GLN

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Mol	Chain	Res	Type
1	D	261	ASN
1	D	275	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 ⓘ

4 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	VTJ	B	301	-	39,40,40	1.62	4 (10%)	52,61,61	1.15	3 (5%)
2	VTJ	A	301	-	39,40,40	1.59	3 (7%)	52,61,61	1.12	4 (7%)
2	VTJ	C	301	-	39,40,40	1.48	3 (7%)	52,61,61	0.98	4 (7%)
2	VTJ	D	301	-	39,40,40	1.74	3 (7%)	52,61,61	0.94	3 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VTJ	B	301	-	-	5/16/37/37	0/6/6/6
2	VTJ	A	301	-	-	5/16/37/37	0/6/6/6
2	VTJ	C	301	-	-	3/16/37/37	0/6/6/6
2	VTJ	D	301	-	-	4/16/37/37	0/6/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	VTJ	C28-N24	9.84	1.55	1.46
2	B	301	VTJ	C28-N24	8.92	1.54	1.46
2	A	301	VTJ	C28-N24	8.74	1.54	1.46
2	C	301	VTJ	C28-N24	8.16	1.54	1.46
2	D	301	VTJ	C25-N24	2.67	1.53	1.47
2	B	301	VTJ	C25-N24	2.54	1.52	1.47
2	A	301	VTJ	C25-N24	2.43	1.52	1.47
2	B	301	VTJ	C23-N24	2.41	1.52	1.47
2	C	301	VTJ	C25-N24	2.38	1.52	1.47
2	A	301	VTJ	C23-N24	2.37	1.52	1.47
2	D	301	VTJ	C23-N24	2.26	1.51	1.47
2	C	301	VTJ	C23-N24	2.20	1.51	1.47
2	B	301	VTJ	C5-C9	2.09	1.49	1.44

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	VTJ	O35-C27-C29	4.81	116.52	108.61
2	A	301	VTJ	O35-C27-C29	4.80	116.51	108.61
2	C	301	VTJ	C25-N24-C28	3.60	108.26	104.02
2	B	301	VTJ	C18-C8-C9	-3.31	123.25	126.66
2	B	301	VTJ	C25-N24-C28	3.30	107.91	104.02
2	A	301	VTJ	C18-C8-C9	-3.23	123.34	126.66
2	D	301	VTJ	O35-C27-C29	2.91	113.40	108.61
2	C	301	VTJ	O35-C27-C29	2.90	113.38	108.61
2	D	301	VTJ	C25-N24-C28	2.71	107.21	104.02
2	A	301	VTJ	C25-N24-C28	2.67	107.17	104.02
2	D	301	VTJ	C18-C8-C9	-2.54	124.05	126.66
2	C	301	VTJ	C11-C10-C9	2.40	119.80	114.92
2	A	301	VTJ	C18-C8-N7	2.12	127.02	122.81
2	C	301	VTJ	C23-N24-C28	-2.10	110.12	112.89

There are no chirality outliers.

All (17) torsion outliers are listed below:

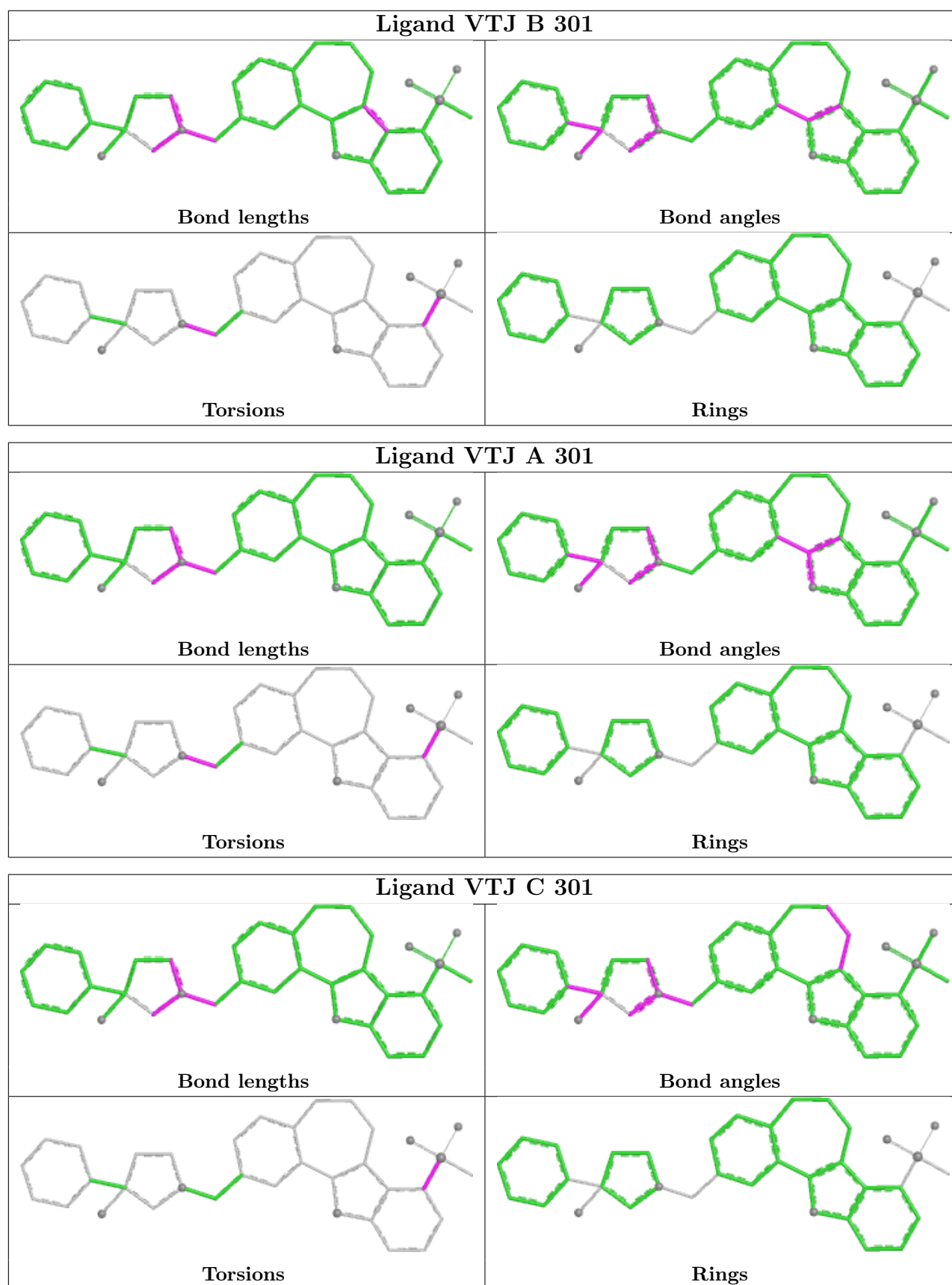
Mol	Chain	Res	Type	Atoms
2	A	301	VTJ	C5-C4-S13-C15
2	A	301	VTJ	C1-C4-S13-C15
2	B	301	VTJ	C5-C4-S13-C15
2	B	301	VTJ	C5-C4-S13-O14
2	B	301	VTJ	C1-C4-S13-C15
2	B	301	VTJ	C20-C23-N24-C25
2	C	301	VTJ	C5-C4-S13-C15
2	C	301	VTJ	C1-C4-S13-C15
2	D	301	VTJ	C5-C4-S13-C15
2	D	301	VTJ	C5-C4-S13-O16
2	D	301	VTJ	C1-C4-S13-C15
2	A	301	VTJ	C20-C23-N24-C25
2	B	301	VTJ	C1-C4-S13-O14
2	A	301	VTJ	C1-C4-S13-O14
2	A	301	VTJ	C5-C4-S13-O14
2	C	301	VTJ	C5-C4-S13-O14
2	D	301	VTJ	C1-C4-S13-O16

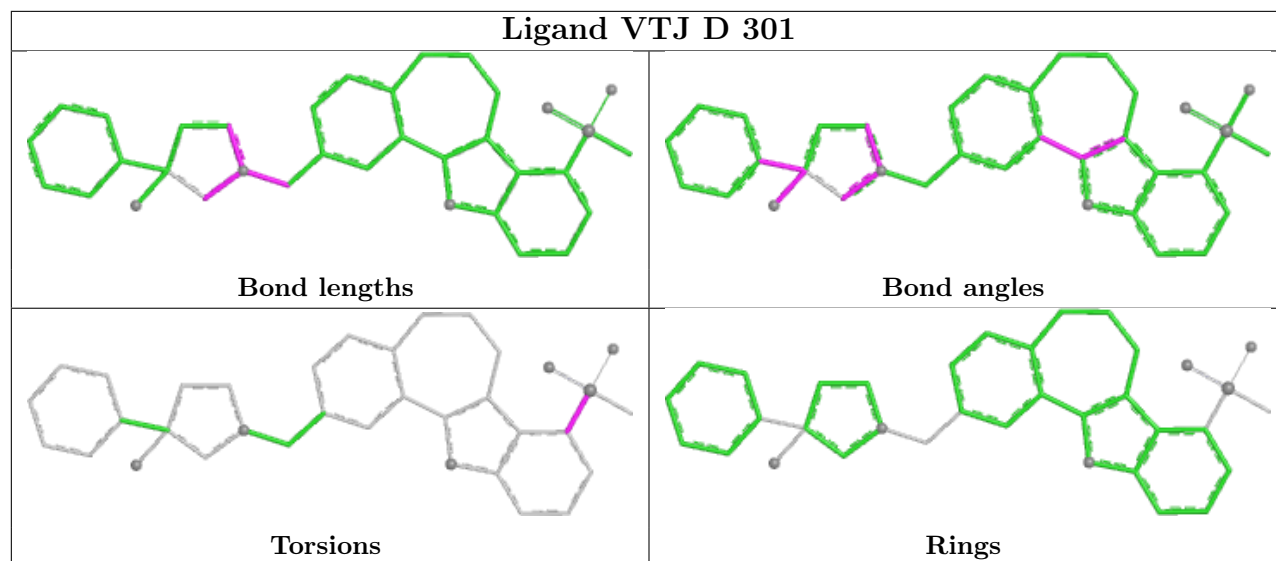
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	VTJ	1	0
2	A	301	VTJ	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	296/316 (93%)	0.60	14 (4%)	36 35	21, 31, 49, 59	0
1	B	296/316 (93%)	0.60	15 (5%)	33 32	20, 31, 50, 62	0
1	C	296/316 (93%)	1.02	26 (8%)	15 14	24, 37, 55, 64	0
1	D	295/316 (93%)	1.11	45 (15%)	5 4	22, 38, 54, 70	0
All	All	1183/1264 (93%)	0.83	100 (8%)	16 15	20, 34, 53, 70	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	VAL	4.9
1	B	298	VAL	4.5
1	C	298	VAL	4.5
1	C	202	GLN	3.9
1	D	30	ARG	3.8
1	D	250	VAL	3.7
1	D	298	VAL	3.7
1	D	174	LYS	3.5
1	D	180	PHE	3.4
1	A	217	LYS	3.3
1	A	295	ASP	3.3
1	A	214	ARG	3.2
1	D	195	VAL	3.1
1	B	214	ARG	3.0
1	B	180	PHE	3.0
1	A	115	THR	3.0
1	D	164	GLN	2.9
1	D	251	VAL	2.9
1	C	214	ARG	2.9
1	C	131	THR	2.9
1	A	104	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	158	ALA	2.8
1	D	198	HIS	2.8
1	C	163	PRO	2.8
1	D	202	GLN	2.8
1	C	185	TYR	2.8
1	A	175	PRO	2.8
1	B	174	LYS	2.7
1	C	182	LEU	2.7
1	A	180	PHE	2.7
1	D	85	GLN	2.7
1	A	296	GLY	2.7
1	B	226	ALA	2.6
1	D	201	PHE	2.6
1	D	249	ARG	2.6
1	B	198	HIS	2.6
1	D	55	ALA	2.6
1	D	161	PRO	2.6
1	B	21	ASP	2.6
1	D	295	ASP	2.6
1	D	193	LYS	2.6
1	A	297	ILE	2.5
1	C	216	LYS	2.5
1	D	56	ARG	2.5
1	C	180	PHE	2.5
1	D	296	GLY	2.5
1	B	295	ASP	2.5
1	D	162	LEU	2.5
1	A	197	LYS	2.5
1	A	198	HIS	2.5
1	D	26	GLU	2.5
1	D	131	THR	2.4
1	C	296	GLY	2.4
1	D	294	PHE	2.4
1	D	227	GLU	2.4
1	D	297	ILE	2.4
1	D	204	ALA	2.4
1	D	21	ASP	2.4
1	B	209	ARG	2.4
1	C	56	ARG	2.4
1	D	224	ALA	2.3
1	D	200	GLY	2.3
1	D	203	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	79	ARG	2.3
1	C	173	GLU	2.3
1	C	85	GLN	2.3
1	C	132	ARG	2.3
1	D	155	GLU	2.3
1	C	16	ILE	2.2
1	B	31	ARG	2.2
1	C	22	LYS	2.2
1	D	128	VAL	2.2
1	B	114	ASP	2.2
1	C	88	TRP	2.2
1	A	30	ARG	2.2
1	C	104	SER	2.2
1	B	217	LYS	2.2
1	D	225	TRP	2.2
1	D	177	GLU	2.1
1	C	97	SER	2.1
1	B	29	ASP	2.1
1	C	21	ASP	2.1
1	C	295	ASP	2.1
1	D	284	VAL	2.1
1	B	175	PRO	2.1
1	C	225	TRP	2.1
1	D	159	LYS	2.1
1	D	130	LEU	2.1
1	D	91	GLN	2.1
1	D	49	VAL	2.1
1	D	183	PHE	2.1
1	D	63	LEU	2.0
1	B	103	ASN	2.0
1	D	175	PRO	2.0
1	C	178	GLU	2.0
1	C	227	GLU	2.0
1	A	199	LEU	2.0
1	C	162	LEU	2.0
1	D	176	ARG	2.0
1	D	156	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

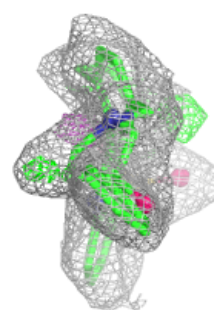
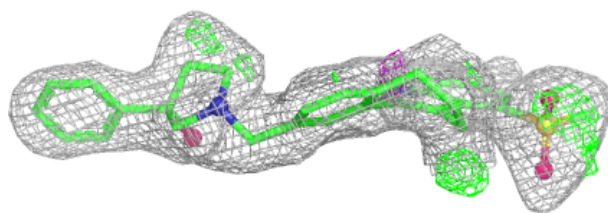
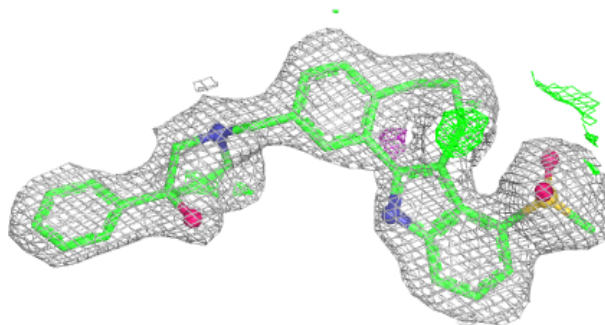
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	VTJ	D	301	35/35	0.86	0.14	38,42,44,45	0
2	VTJ	C	301	35/35	0.88	0.13	37,41,45,45	0
2	VTJ	B	301	35/35	0.90	0.12	28,35,39,40	0
2	VTJ	A	301	35/35	0.93	0.09	27,30,34,39	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.

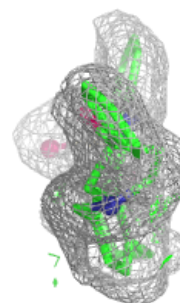
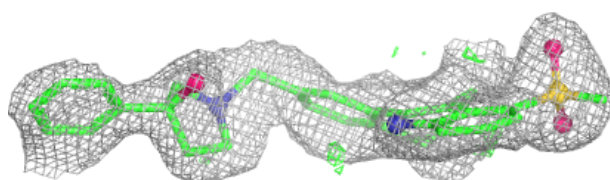
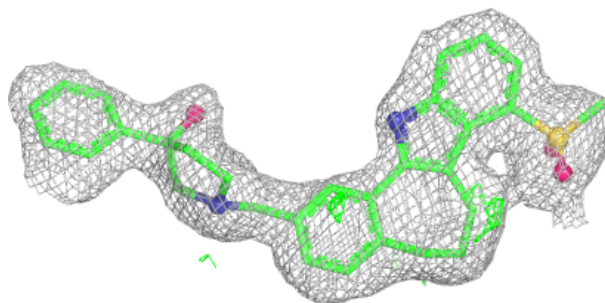
Electron density around VTJ D 301:

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

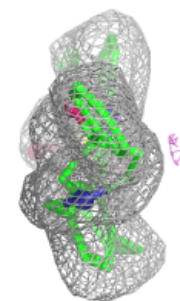
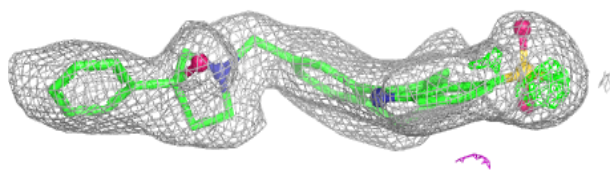
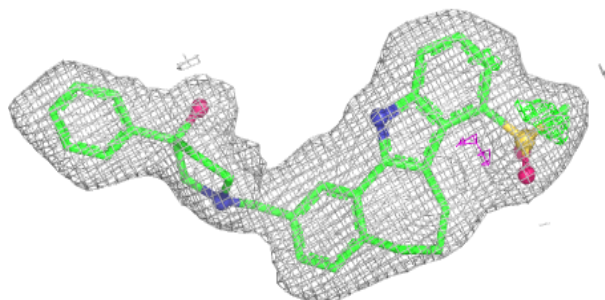


Electron density around VTJ C 301:

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

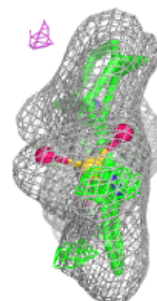
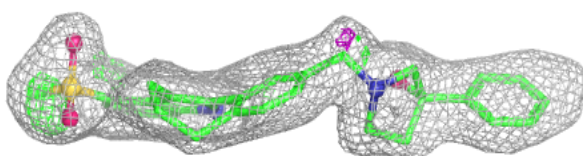
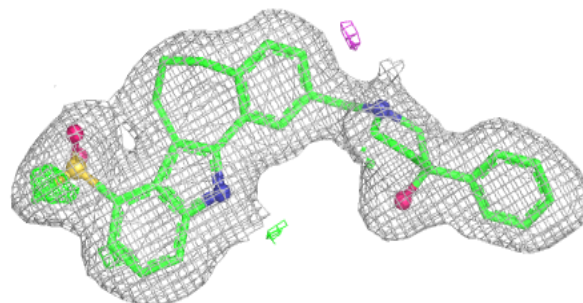
**Electron density around VTJ B 301:**

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



Electron density around VTJ A 301:

$2mF_o-DF_c$ (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.