



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:36 PM UTC

PDB ID : 4PA6 / pdb_00004pa6
Title : Structure of NavMS pore and C-terminal domain crystallised in the presence of channel blocking compound
Authors : Naylor, C.E.; Bagneris, C.; Wallace, B.A.
Deposited on : 2014-04-07
Resolution : 3.36 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

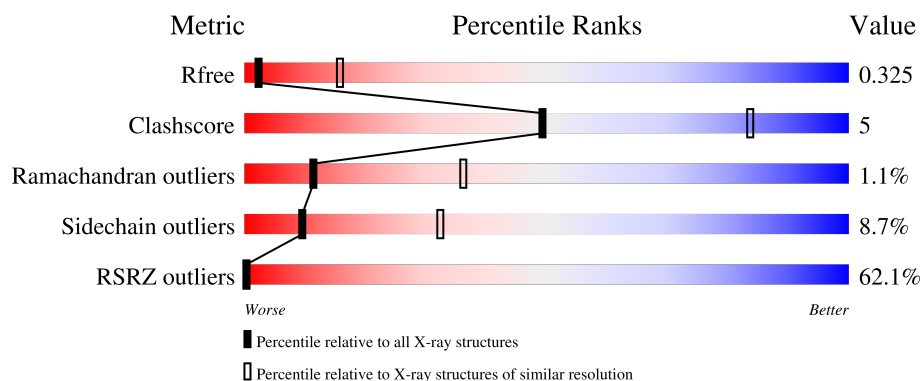
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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 $\leq 5\%$. 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	149	40% 47%15%38%
1	B	149	40% 42%18%40%
1	C	149	38% 47%13%39%
1	D	149	34% 45%14%39%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2950 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.

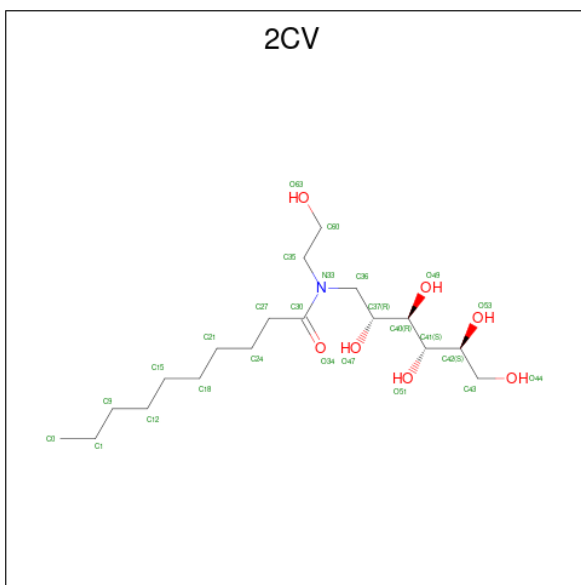
- Molecule 1 is a protein called Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	S	0	0	0
			718	488	106	119	5			
1	B	90	Total	C	N	O	S	0	0	0
			711	483	104	119	5			
1	C	91	Total	C	N	O	S	0	0	0
			715	485	105	120	5			
1	D	91	Total	C	N	O	S	0	0	0
			712	482	105	120	5			

There are 16 discrepancies between the modelled and reference sequences:

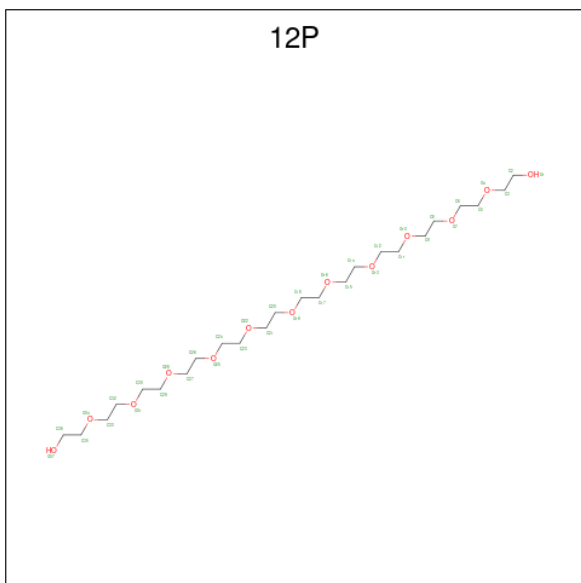
Chain	Residue	Modelled	Actual	Comment	Reference
A	126	GLY	-	expression tag	UNP A0L5S6
A	127	SER	-	expression tag	UNP A0L5S6
A	128	HIS	-	expression tag	UNP A0L5S6
A	129	MET	-	expression tag	UNP A0L5S6
B	126	GLY	-	expression tag	UNP A0L5S6
B	127	SER	-	expression tag	UNP A0L5S6
B	128	HIS	-	expression tag	UNP A0L5S6
B	129	MET	-	expression tag	UNP A0L5S6
C	126	GLY	-	expression tag	UNP A0L5S6
C	127	SER	-	expression tag	UNP A0L5S6
C	128	HIS	-	expression tag	UNP A0L5S6
C	129	MET	-	expression tag	UNP A0L5S6
D	126	GLY	-	expression tag	UNP A0L5S6
D	127	SER	-	expression tag	UNP A0L5S6
D	128	HIS	-	expression tag	UNP A0L5S6
D	129	MET	-	expression tag	UNP A0L5S6

- Molecule 2 is HEGA-10 (CCD ID: 2CV) (formula: $C_{18}H_{37}NO_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 15	C 10	N 1	O 4	0	0
2	B	1	Total 15	C 10	N 1	O 4	0	0
2	C	1	Total 15	C 10	N 1	O 4	0	0
2	D	1	Total 15	C 10	N 1	O 4	0	0

- Molecule 3 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: $C_{24}H_{50}O_{13}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		

- 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		
4	C	2	Total	Na	0	0
			2	2		

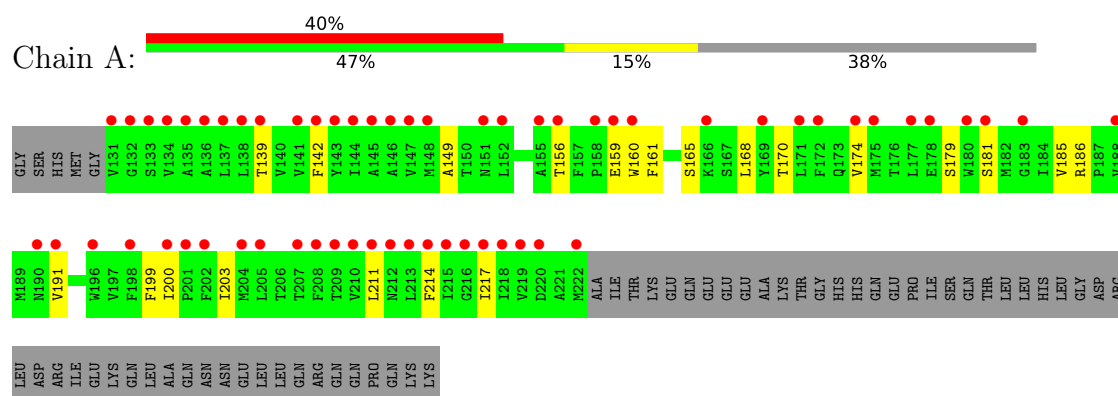
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	2	Total	O	0	0
			2	2		
5	C	5	Total	O	0	0
			5	5		
5	D	6	Total	O	0	0
			6	6		

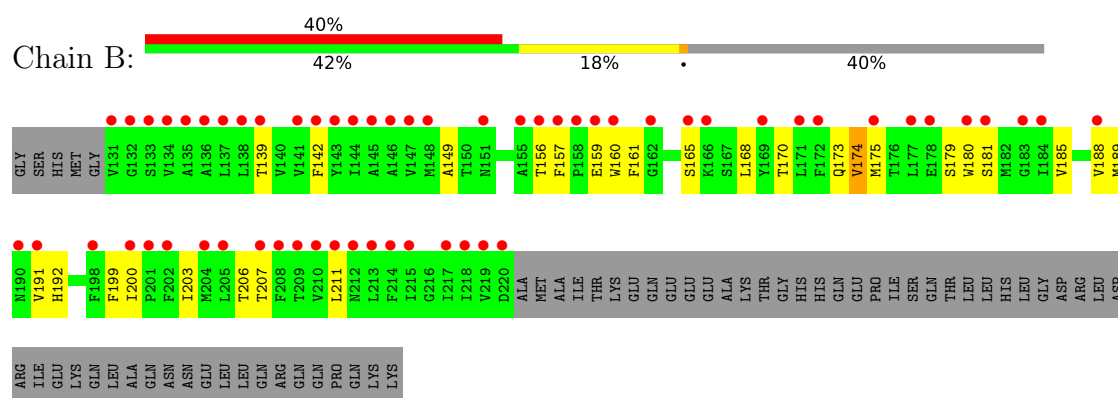
3 Residue-property plots

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.

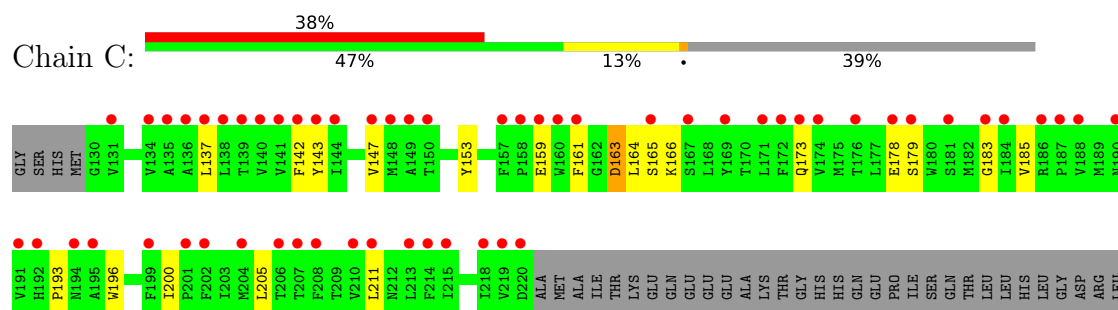
• Molecule 1: Ion transport protein



• Molecule 1: Ion transport protein

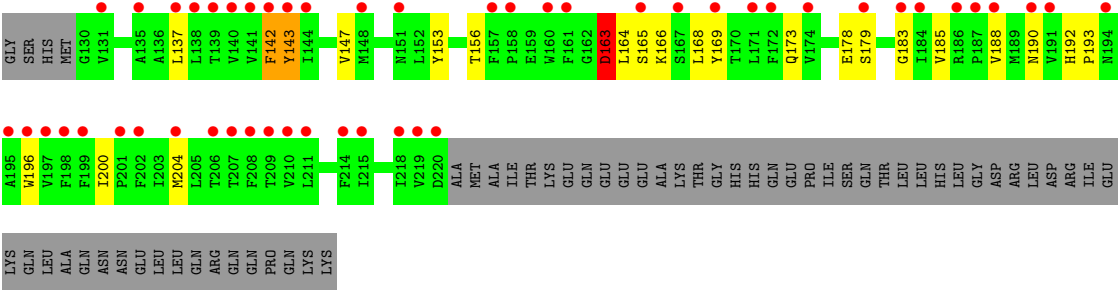


• Molecule 1: Ion transport protein



ASP	ARG	ILE	GLU	LYS	GLN	LEU	ALA	GLN	ASN	GLU	LEU	GLN	ARG	GLN	PRO	GLN	LYS
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● Molecule 1: Ion transport protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	79.93Å 324.57Å 79.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.77 – 3.36 44.77 – 3.36	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.77-3.36) 99.6 (44.77-3.36)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.302 , 0.342 0.294 , 0.325	Depositor DCC
R_{free} test set	792 reflections (1.77%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	1.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	2950	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3499e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 2CV, NA, 12P

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	0.87	0/740	1.54	3/1015 (0.3%)
1	B	0.87	0/733	1.53	3/1005 (0.3%)
1	C	0.90	0/737	1.53	7/1010 (0.7%)
1	D	0.91	0/734	1.52	7/1006 (0.7%)
All	All	0.89	0/2944	1.53	20/4036 (0.5%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	PHE	N-CA-C	7.89	119.96	111.36
1	B	199	PHE	N-CA-C	7.80	119.86	111.36
1	A	200	ILE	N-CA-CB	7.49	116.29	110.45
1	B	200	ILE	N-CA-CB	6.53	115.55	110.45
1	D	163	ASP	CA-CB-CG	6.10	118.70	112.60
1	B	191	VAL	N-CA-C	-5.86	106.99	111.62
1	A	191	VAL	N-CA-C	-5.70	107.11	111.62
1	D	164	LEU	CA-C-N	5.29	127.32	120.44
1	D	164	LEU	C-N-CA	5.29	127.32	120.44
1	C	185	VAL	N-CA-C	5.22	115.43	110.42
1	C	163	ASP	CA-CB-CG	5.21	117.81	112.60
1	D	185	VAL	N-CA-C	5.21	115.42	110.42
1	C	161	PHE	CA-C-N	5.20	125.87	119.99
1	C	161	PHE	C-N-CA	5.20	125.87	119.99
1	D	193	PRO	N-CA-C	5.13	121.25	113.81
1	C	164	LEU	CA-C-N	5.09	127.06	120.44
1	C	164	LEU	C-N-CA	5.09	127.06	120.44
1	C	193	PRO	N-CA-C	5.07	121.16	113.81
1	D	143	TYR	CA-C-N	5.06	126.94	120.56
1	D	143	TYR	C-N-CA	5.06	126.94	120.56

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	718	0	726	8	0
1	B	711	0	721	12	0
1	C	715	0	724	4	0
1	D	712	0	715	8	0
2	A	15	0	16	1	0
2	B	15	0	16	0	0
2	C	15	0	16	2	0
2	D	15	0	16	0	0
3	A	16	0	21	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	5	0	0	0	0
5	D	6	0	0	0	0
All	All	2950	0	2971	32	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 (32) 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)
2:C:301:2CV:H212	1:D:169:TYR:HB2	1.76	0.68
1:C:196:TRP:HB2	1:C:200:ILE:HD12	1.88	0.56
1:C:179:SER:HB3	1:C:183:GLY:HA3	1.89	0.55
2:C:301:2CV:H37	2:C:301:2CV:O34	2.07	0.55
1:A:160:TRP:HB3	1:A:170:THR:HG21	1.89	0.55
1:D:179:SER:HB3	1:D:183:GLY:HA3	1.88	0.54
1:D:196:TRP:HB2	1:D:200:ILE:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:TRP:HB3	1:B:170:THR:HG21	1.91	0.53
1:A:149:ALA:HB1	1:A:161:PHE:CD1	2.45	0.52
1:B:181:SER:HA	1:B:185:VAL:HB	1.96	0.47
1:B:157:PHE:CZ	1:B:188:VAL:HA	2.51	0.46
1:B:149:ALA:HB1	1:B:161:PHE:CD1	2.52	0.45
1:C:163:ASP:H	1:C:166:LYS:HD2	1.80	0.45
1:B:175:MET:HG3	1:B:206:THR:HB	1.99	0.44
1:A:174:VAL:HG13	1:A:203:ILE:HD11	1.98	0.44
1:B:175:MET:O	1:B:207:THR:HG22	2.18	0.44
1:A:165:SER:HA	1:A:168:LEU:HD12	2.00	0.43
1:B:165:SER:HA	1:B:168:LEU:HD12	2.01	0.43
1:A:214:PHE:HA	1:A:217:ILE:HD12	2.01	0.43
1:C:143:TYR:O	1:C:147:VAL:HG23	2.18	0.43
1:B:180:TRP:HE3	1:B:185:VAL:HG21	1.84	0.42
1:A:181:SER:HB3	1:B:173:GLN:HG3	2.00	0.42
1:A:181:SER:HA	1:A:185:VAL:HB	2.01	0.42
1:D:143:TYR:O	1:D:147:VAL:HG23	2.19	0.42
2:A:301:2CV:O34	2:A:301:2CV:H37	2.19	0.42
1:D:188:VAL:HG13	1:D:192:HIS:HD2	1.85	0.41
1:D:200:ILE:HG22	1:D:204:MET:HE2	2.01	0.41
1:D:163:ASP:H	1:D:166:LYS:HD2	1.86	0.41
1:B:174:VAL:HG13	1:B:203:ILE:HD11	2.03	0.41
1:B:189:MET:HA	1:B:192:HIS:O	2.21	0.40
1:D:142:PHE:HD2	1:D:168:LEU:HD23	1.87	0.40
1:A:186:ARG:NH2	1:B:170:THR:HG23	2.36	0.40

There are no symmetry-related clashes.

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	90/149 (60%)	81 (90%)	8 (9%)	1 (1%)	11 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	88/149 (59%)	81 (92%)	6 (7%)	1 (1%)	11	36
1	C	89/149 (60%)	83 (93%)	5 (6%)	1 (1%)	11	36
1	D	89/149 (60%)	83 (93%)	5 (6%)	1 (1%)	11	36
All	All	356/596 (60%)	328 (92%)	24 (7%)	4 (1%)	11	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	SER
1	B	179	SER
1	C	178	GLU
1	D	178	GLU

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	77/129 (60%)	72 (94%)	5 (6%)	15	42
1	B	78/129 (60%)	72 (92%)	6 (8%)	12	37
1	C	78/129 (60%)	70 (90%)	8 (10%)	7	25
1	D	77/129 (60%)	69 (90%)	8 (10%)	7	24
All	All	310/516 (60%)	283 (91%)	27 (9%)	9	32

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

Mol	Chain	Res	Type
1	A	139	THR
1	A	142	PHE
1	A	156	THR
1	A	159	GLU
1	A	211	LEU
1	B	139	THR
1	B	142	PHE

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Mol	Chain	Res	Type
1	B	156	THR
1	B	159	GLU
1	B	174	VAL
1	B	211	LEU
1	C	137	LEU
1	C	142	PHE
1	C	153	TYR
1	C	159	GLU
1	C	165	SER
1	C	173	GLN
1	C	205	LEU
1	C	211	LEU
1	D	137	LEU
1	D	142	PHE
1	D	153	TYR
1	D	156	THR
1	D	163	ASP
1	D	165	SER
1	D	173	GLN
1	D	190	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	194	ASN
1	C	212	ASN
1	D	192	HIS
1	D	194	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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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
2	2CV	B	301	-	14,14,25	0.23	0	16,16,30	0.85	1 (6%)
3	12P	A	302	-	15,15,36	0.16	0	14,14,35	0.11	0
2	2CV	A	301	-	14,14,25	0.24	0	16,16,30	1.16	2 (12%)
2	2CV	D	300	-	14,14,25	0.25	0	16,16,30	0.64	0
2	2CV	C	301	-	14,14,25	0.26	0	16,16,30	1.64	2 (12%)

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	2CV	B	301	-	-	0/17/17/34	-
3	12P	A	302	-	-	5/13/13/34	-
2	2CV	A	301	-	-	5/17/17/34	-
2	2CV	D	300	-	-	2/17/17/34	-
2	2CV	C	301	-	-	7/17/17/34	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	2CV	C37-C36-N33	4.60	118.12	113.10
2	C	301	2CV	C35-N33-C36	-4.28	111.30	116.14
2	A	301	2CV	C37-C36-N33	3.59	117.02	113.10
2	B	301	2CV	C37-C36-N33	2.70	116.05	113.10
2	A	301	2CV	C35-N33-C36	-2.42	113.40	116.14

There are no chirality outliers.

All (19) torsion outliers are listed below:

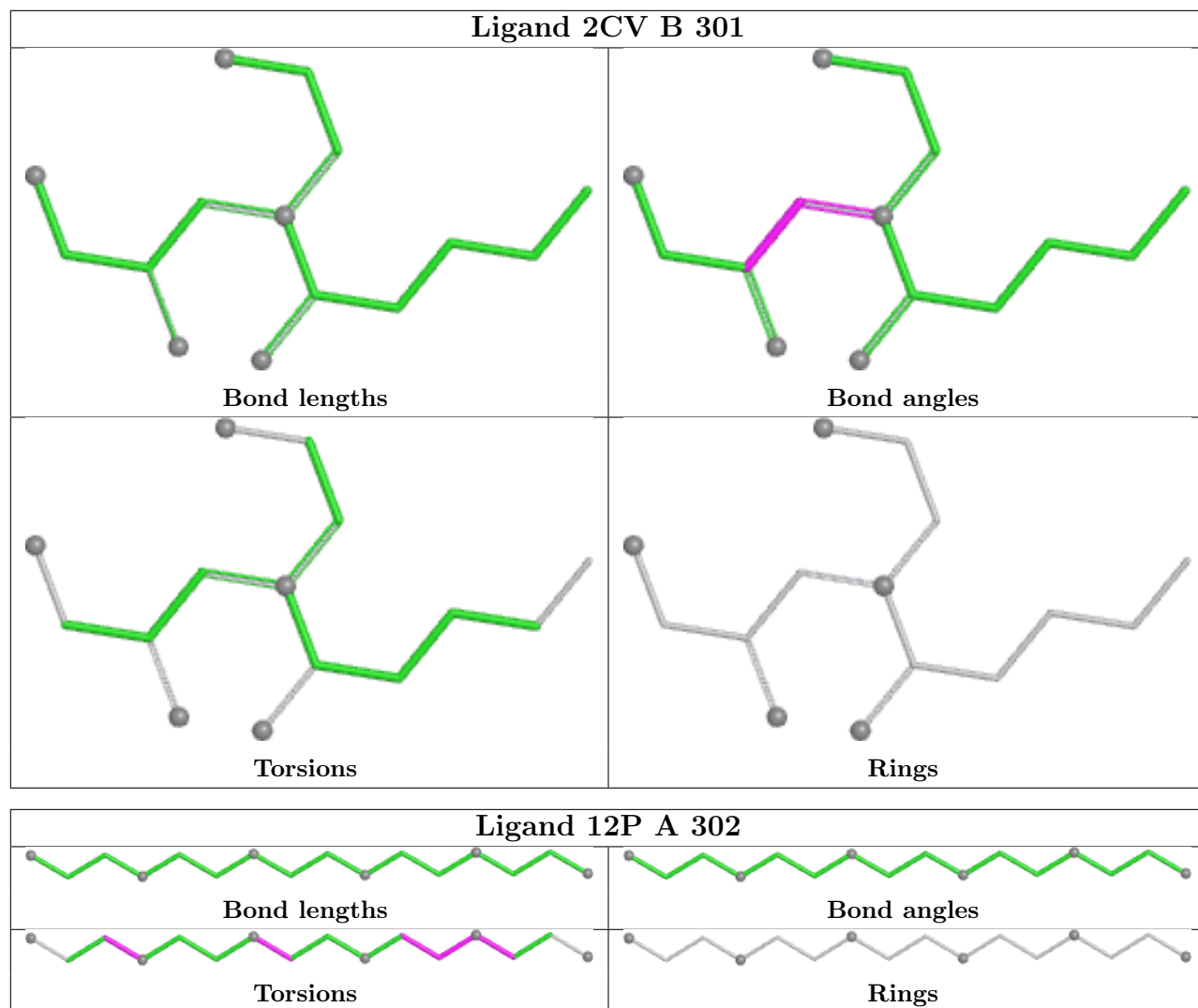
Mol	Chain	Res	Type	Atoms
2	A	301	2CV	N33-C36-C37-C40
2	A	301	2CV	N33-C36-C37-O47
2	C	301	2CV	C37-C36-N33-C30
2	C	301	2CV	C37-C36-N33-C35
2	C	301	2CV	N33-C36-C37-C40
2	C	301	2CV	C36-C37-C40-O49
2	C	301	2CV	O47-C37-C40-O49
2	D	300	2CV	N33-C35-C60-O63
2	A	301	2CV	C37-C36-N33-C30
2	C	301	2CV	N33-C36-C37-O47
2	A	301	2CV	C37-C36-N33-C35
2	C	301	2CV	N33-C35-C60-O63
3	A	302	12P	C9-C8-O7-C6
3	A	302	12P	C15-C14-O13-C12
2	D	300	2CV	O47-C37-C40-O49
3	A	302	12P	O10-C11-C12-O13
3	A	302	12P	C2-C3-O4-C5
3	A	302	12P	C11-C12-O13-C14
2	A	301	2CV	C36-C37-C40-O49

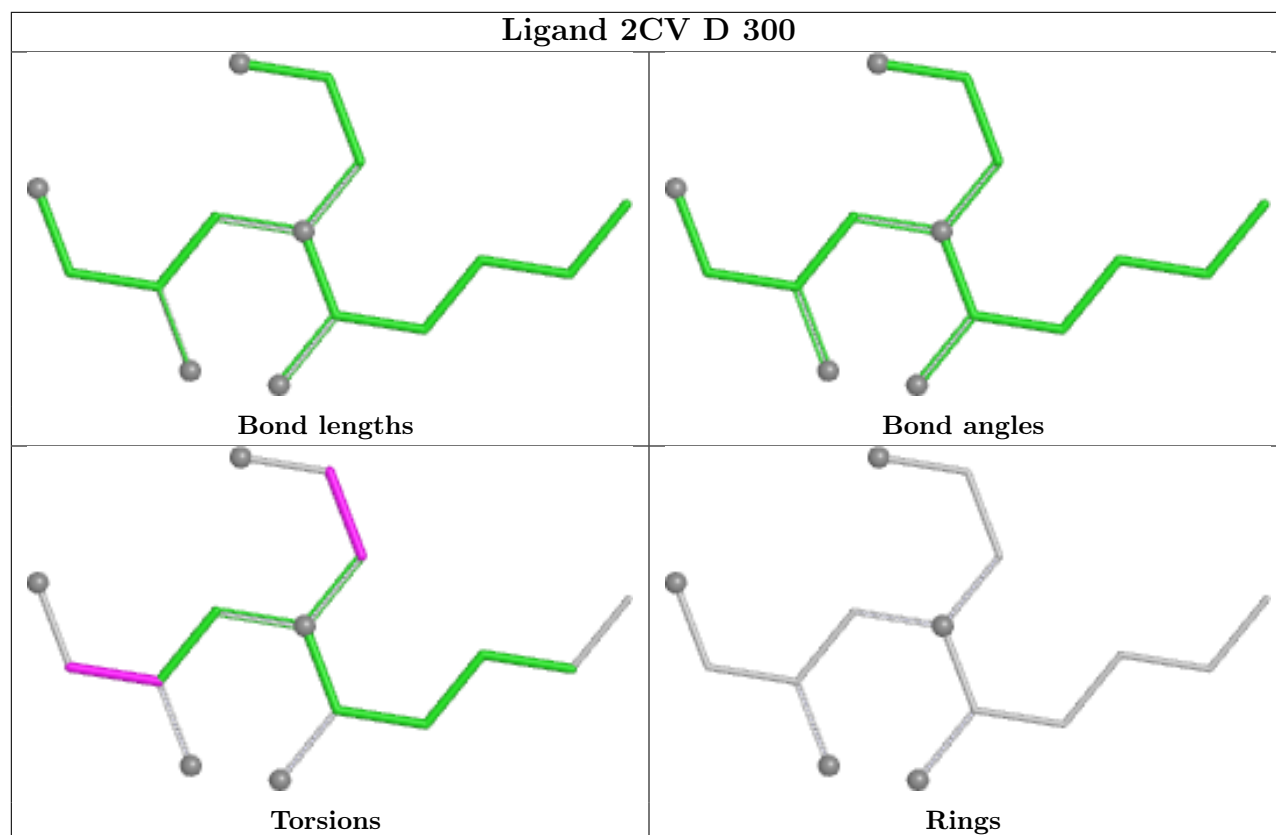
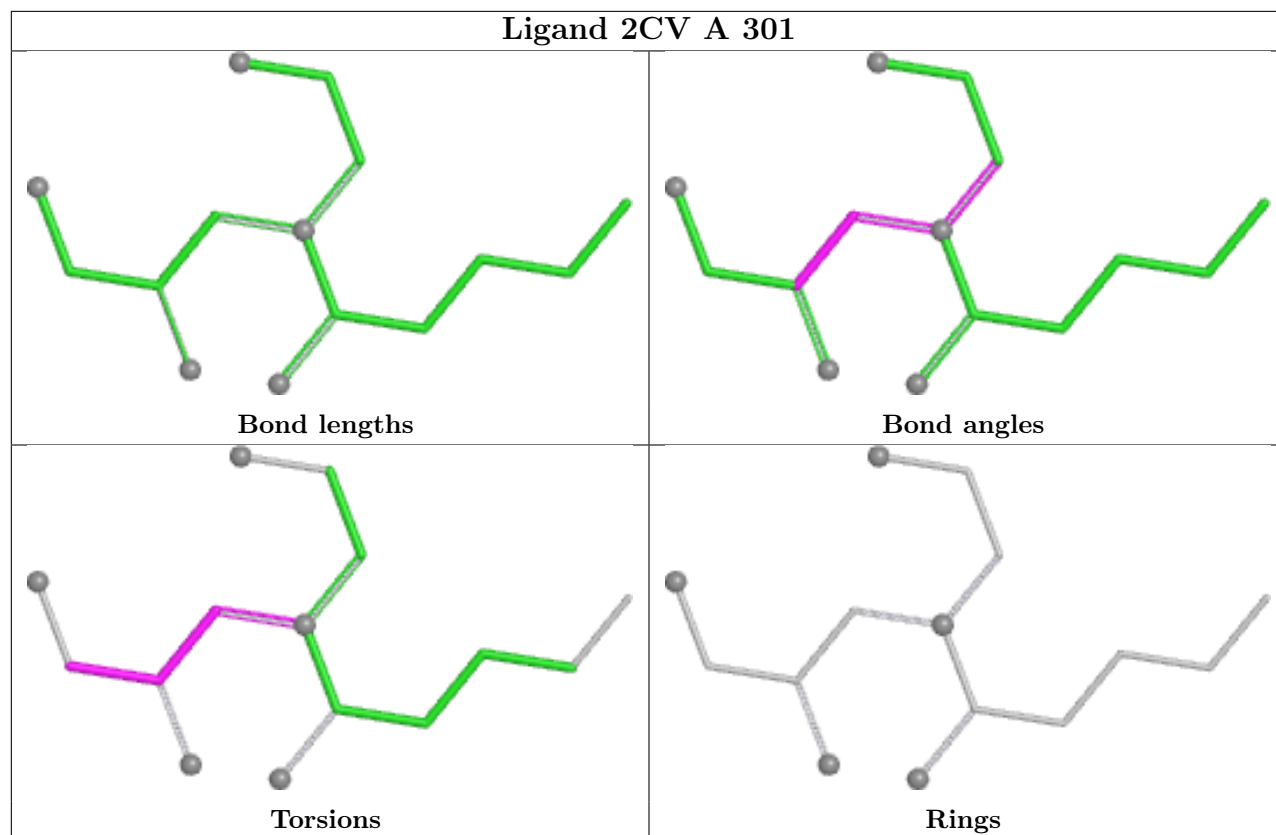
There are no ring outliers.

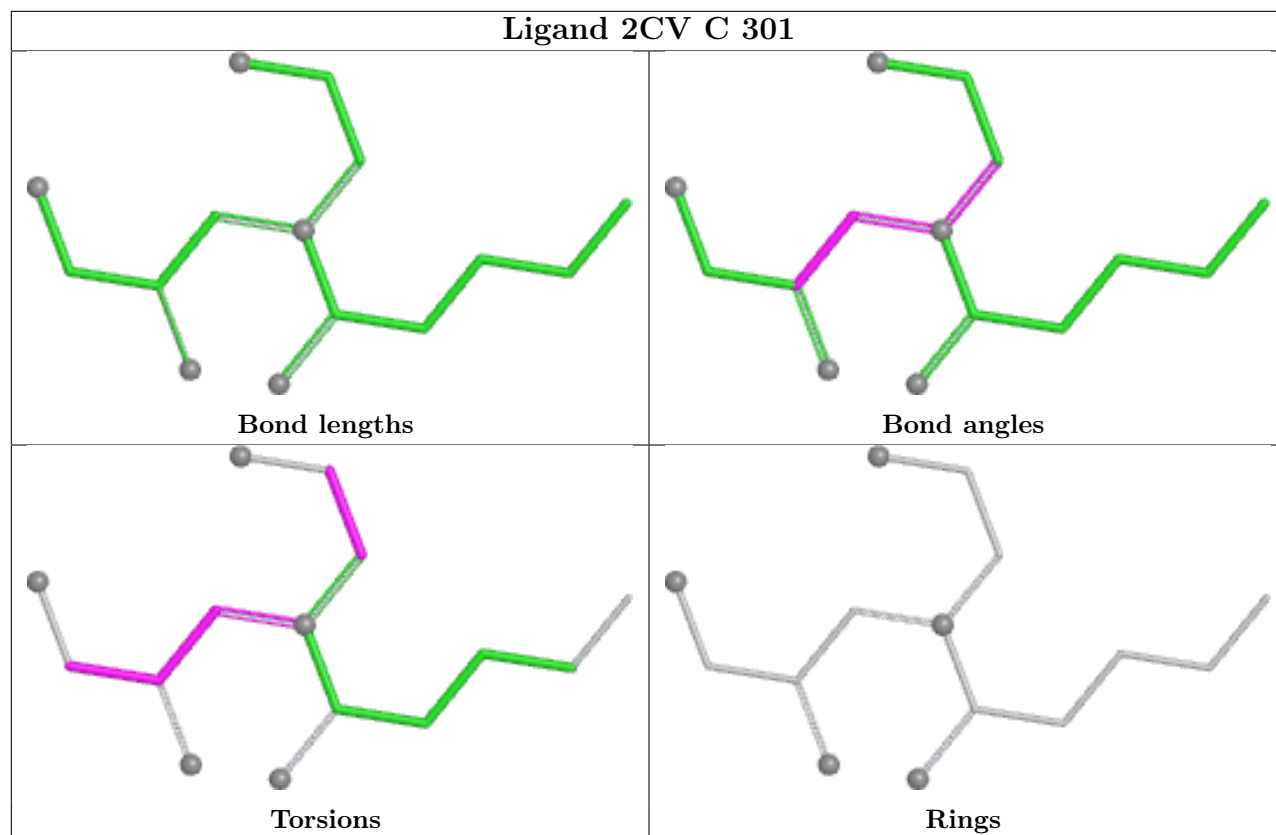
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	2CV	1	0
2	C	301	2CV	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 ⓘ

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	92/149 (61%)	2.76	60 (65%) 0 0	44, 59, 140, 214	0
1	B	90/149 (60%)	2.76	59 (65%) 0 0	45, 60, 138, 203	0
1	C	91/149 (61%)	2.41	57 (62%) 0 0	43, 62, 130, 197	0
1	D	91/149 (61%)	2.36	50 (54%) 0 0	43, 60, 134, 201	0
All	All	364/596 (61%)	2.57	226 (62%) 0 0	43, 60, 140, 214	0

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	140	VAL	7.9
1	C	140	VAL	7.2
1	B	207	THR	7.1
1	A	143	TYR	5.7
1	D	144	ILE	5.7
1	A	222	MET	5.6
1	A	131	VAL	5.6
1	B	143	TYR	5.5
1	D	204	MET	5.4
1	B	138	LEU	5.4
1	C	188	VAL	5.4
1	C	144	ILE	5.3
1	A	217	ILE	5.3
1	A	137	LEU	5.2
1	B	211	LEU	5.2
1	C	220	ASP	5.2
1	A	214	PHE	5.1
1	B	137	LEU	5.1
1	A	132	GLY	5.0
1	D	188	VAL	5.0
1	B	214	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	133	SER	4.9
1	A	135	ALA	4.8
1	A	211	LEU	4.8
1	B	131	VAL	4.8
1	D	143	TYR	4.8
1	C	191	VAL	4.8
1	D	191	VAL	4.8
1	B	159	GLU	4.7
1	D	220	ASP	4.7
1	A	190	ASN	4.7
1	B	135	ALA	4.7
1	C	204	MET	4.6
1	A	138	LEU	4.6
1	B	210	VAL	4.6
1	A	133	SER	4.5
1	B	212	ASN	4.5
1	A	207	THR	4.5
1	B	217	ILE	4.4
1	B	158	PRO	4.4
1	D	195	ALA	4.3
1	A	212	ASN	4.3
1	B	204	MET	4.3
1	D	160	TRP	4.2
1	A	220	ASP	4.2
1	D	148	MET	4.2
1	C	195	ALA	4.2
1	A	158	PRO	4.2
1	B	215	ILE	4.2
1	C	160	TRP	4.2
1	C	143	TYR	4.1
1	A	210	VAL	4.1
1	B	148	MET	4.1
1	A	198	PHE	4.1
1	A	141	VAL	4.1
1	C	148	MET	4.0
1	B	208	PHE	4.0
1	C	210	VAL	4.0
1	A	218	ILE	4.0
1	C	179	SER	4.0
1	A	148	MET	3.9
1	D	138	LEU	3.9
1	B	198	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	157	PHE	3.8
1	A	215	ILE	3.8
1	D	210	VAL	3.8
1	B	220	ASP	3.7
1	A	139	THR	3.7
1	C	190	ASN	3.7
1	A	213	LEU	3.7
1	A	208	PHE	3.7
1	B	132	GLY	3.7
1	C	157	PHE	3.7
1	A	169	TYR	3.6
1	B	141	VAL	3.6
1	D	141	VAL	3.6
1	B	139	THR	3.6
1	A	204	MET	3.6
1	B	190	ASN	3.6
1	C	211	LEU	3.6
1	C	161	PHE	3.6
1	A	134	VAL	3.6
1	B	134	VAL	3.6
1	B	205	LEU	3.5
1	D	179	SER	3.5
1	B	213	LEU	3.5
1	B	136	ALA	3.5
1	C	207	THR	3.4
1	B	160	TRP	3.4
1	B	169	TYR	3.4
1	B	166	LYS	3.4
1	D	207	THR	3.4
1	B	146	ALA	3.3
1	C	158	PRO	3.3
1	C	186	ARG	3.3
1	B	147	VAL	3.3
1	C	165	SER	3.3
1	B	218	ILE	3.3
1	A	136	ALA	3.3
1	A	166	LYS	3.2
1	C	138	LEU	3.2
1	C	184	ILE	3.2
1	D	131	VAL	3.2
1	A	181	SER	3.2
1	B	175	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	171	LEU	3.2
1	D	169	TYR	3.2
1	A	205	LEU	3.1
1	C	141	VAL	3.1
1	D	208	PHE	3.1
1	C	201	PRO	3.1
1	B	155	ALA	3.1
1	A	191	VAL	3.1
1	C	218	ILE	3.1
1	B	171	LEU	3.1
1	B	209	THR	3.1
1	C	178	GLU	3.1
1	D	206	THR	3.0
1	A	147	VAL	3.0
1	C	206	THR	3.0
1	D	187	PRO	3.0
1	D	186	ARG	3.0
1	A	146	ALA	2.9
1	B	145	ALA	2.9
1	C	169	TYR	2.9
1	B	142	PHE	2.9
1	C	208	PHE	2.9
1	D	158	PRO	2.9
1	D	201	PRO	2.9
1	D	219	VAL	2.9
1	C	131	VAL	2.9
1	D	184	ILE	2.9
1	B	151	ASN	2.8
1	A	152	LEU	2.8
1	A	216	GLY	2.8
1	C	142	PHE	2.8
1	A	209	THR	2.8
1	A	145	ALA	2.7
1	B	219	VAL	2.7
1	C	219	VAL	2.7
1	C	137	LEU	2.7
1	B	181	SER	2.7
1	A	155	ALA	2.7
1	D	137	LEU	2.7
1	D	215	ILE	2.7
1	A	142	PHE	2.7
1	C	214	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	214	PHE	2.7
1	B	184	ILE	2.6
1	A	160	TRP	2.6
1	C	202	PHE	2.6
1	C	187	PRO	2.6
1	A	183	GLY	2.6
1	B	177	LEU	2.6
1	C	135	ALA	2.6
1	D	209	THR	2.6
1	A	175	MET	2.6
1	A	219	VAL	2.6
1	B	191	VAL	2.6
1	A	172	PHE	2.5
1	B	172	PHE	2.5
1	B	165	SER	2.5
1	C	134	VAL	2.5
1	D	202	PHE	2.5
1	D	167	SER	2.5
1	B	144	ILE	2.5
1	D	161	PHE	2.5
1	C	183	GLY	2.5
1	A	188	VAL	2.5
1	A	196	TRP	2.5
1	A	159	GLU	2.5
1	D	211	LEU	2.5
1	D	197	VAL	2.5
1	D	135	ALA	2.4
1	D	142	PHE	2.4
1	C	139	THR	2.4
1	D	190	ASN	2.4
1	D	183	GLY	2.4
1	B	183	GLY	2.3
1	B	201	PRO	2.3
1	B	162	GLY	2.3
1	C	150	THR	2.3
1	A	151	ASN	2.3
1	A	177	LEU	2.3
1	A	178	GLU	2.3
1	C	181	SER	2.3
1	C	199	PHE	2.3
1	D	165	SER	2.3
1	D	199	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	194	ASN	2.3
1	C	136	ALA	2.2
1	A	156	THR	2.2
1	D	194	ASN	2.2
1	A	180	TRP	2.2
1	C	172	PHE	2.2
1	C	173	GLN	2.2
1	A	200	ILE	2.2
1	C	215	ILE	2.2
1	D	218	ILE	2.2
1	C	149	ALA	2.2
1	C	192	HIS	2.2
1	C	167	SER	2.2
1	D	151	ASN	2.1
1	A	174	VAL	2.1
1	D	196	TRP	2.1
1	B	156	THR	2.1
1	C	171	LEU	2.1
1	A	201	PRO	2.1
1	A	202	PHE	2.1
1	B	157	PHE	2.1
1	D	172	PHE	2.1
1	D	198	PHE	2.1
1	B	188	VAL	2.1
1	C	147	VAL	2.1
1	A	144	ILE	2.1
1	B	202	PHE	2.1
1	D	171	LEU	2.1
1	D	139	THR	2.1
1	D	174	VAL	2.1
1	C	176	THR	2.1
1	B	178	GLU	2.1
1	B	200	ILE	2.0
1	B	180	TRP	2.0
1	C	159	GLU	2.0
1	C	174	VAL	2.0
1	C	213	LEU	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](#)

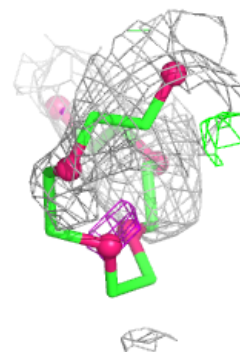
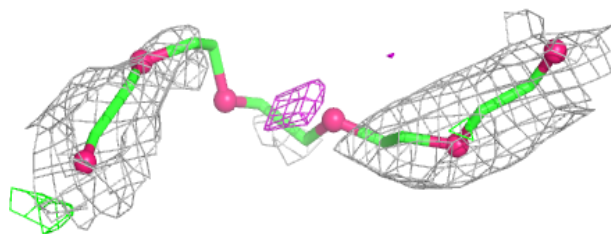
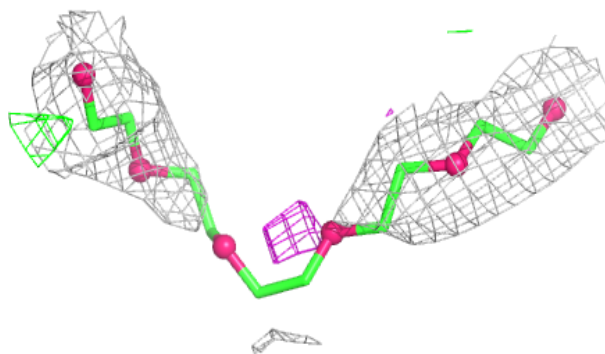
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	12P	A	302	16/37	0.64	0.35	74,85,89,89	0
2	2CV	D	300	15/26	0.70	0.35	86,92,95,97	0
2	2CV	B	301	15/26	0.70	0.32	92,98,103,106	0
2	2CV	C	301	15/26	0.72	0.37	89,98,107,109	0
2	2CV	A	301	15/26	0.75	0.31	97,102,104,104	0
4	NA	B	302	1/1	0.99	0.49	51,51,51,51	1
4	NA	C	302	1/1	0.99	0.51	50,50,50,50	1
4	NA	C	303	1/1	0.99	0.50	54,54,54,54	1
4	NA	A	303	1/1	1.00	0.51	52,52,52,52	1

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.

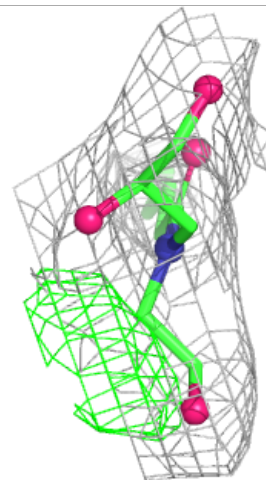
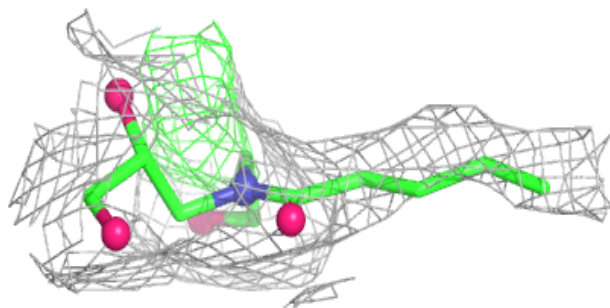
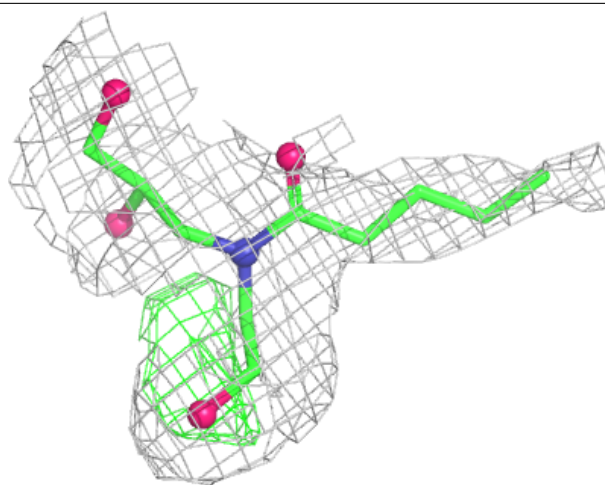
Electron density around 12P A 302:

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



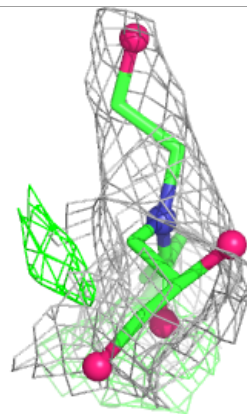
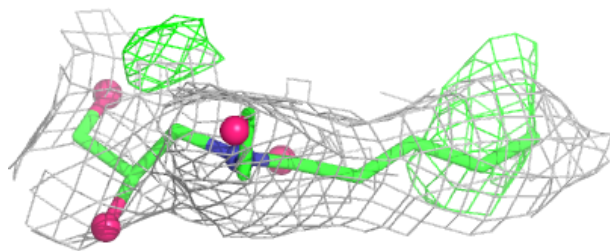
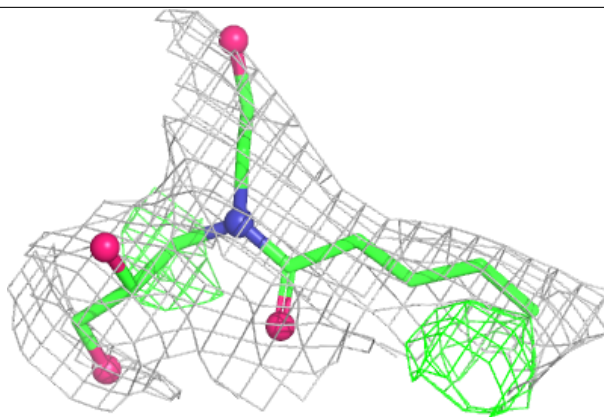
Electron density around 2CV D 300:

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



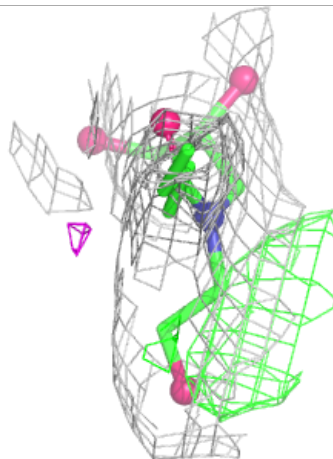
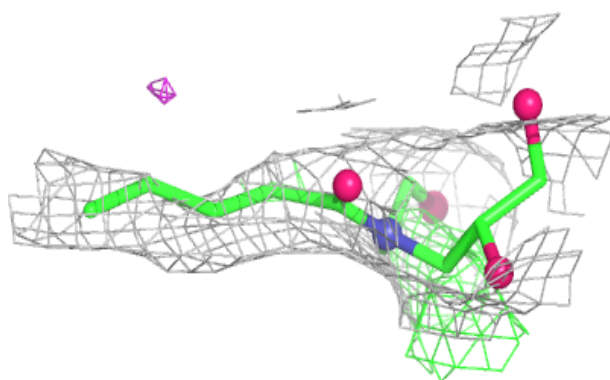
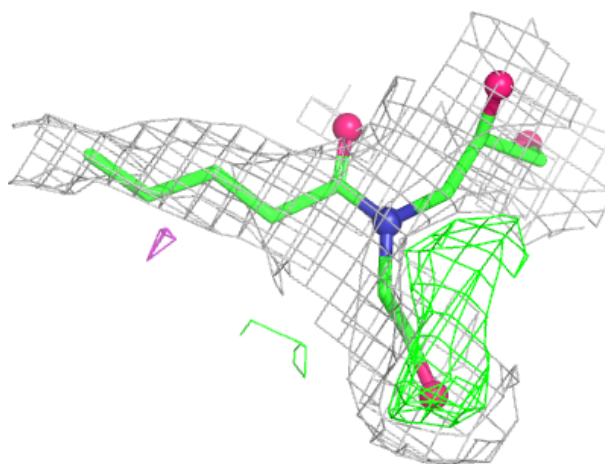
Electron density around 2CV B 301:

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



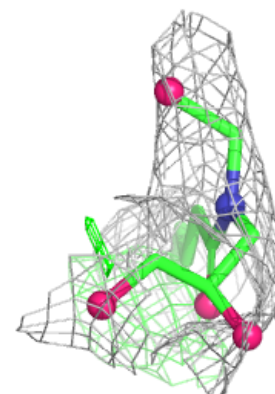
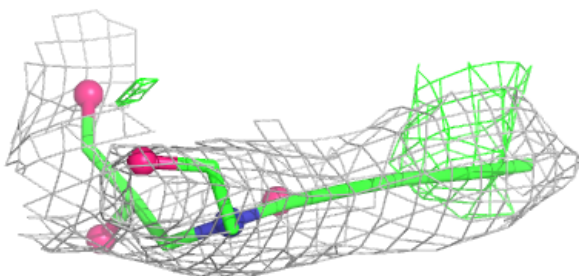
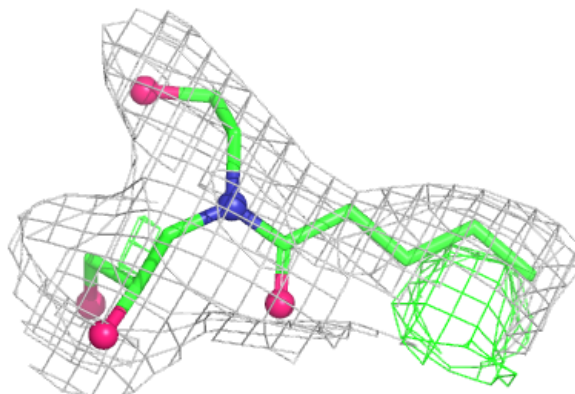
Electron density around 2CV C 301:

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



Electron density around 2CV 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 ⓘ

There are no such residues in this entry.