



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:31 PM UTC

PDB ID : 2YCW / pdb_00002ycw
Title : TURKEY BETA1 ADRENERGIC RECEPTOR WITH STABILISING MUTATIONS AND BOUND ANTAGONIST CARAZOLOL
Authors : Moukhametzianov, R.; Warne, T.; Edwards, P.C.; Serrano-Vega, M.J.; Leslie, A.G.W.; Tate, C.G.; Schertler, G.F.X.
Deposited on : 2011-03-17
Resolution : 3.00 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

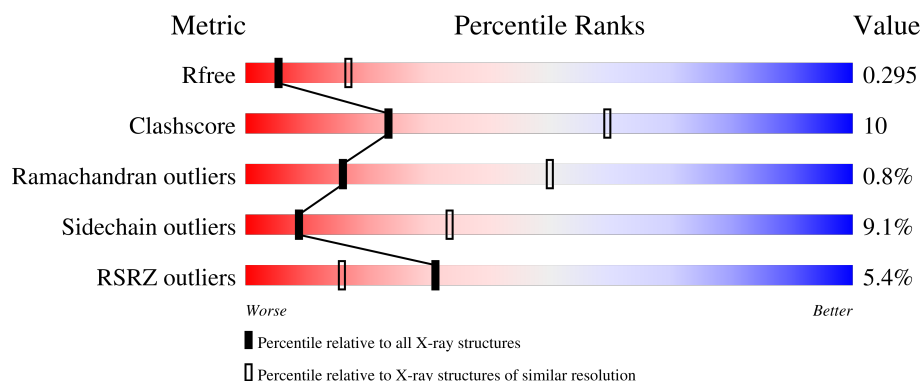
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	313	
1	B	313	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4882 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 BETA-1 ADRENERGIC RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2369	1562	395	392	20			
1	B	297	Total	C	N	O	S	0	0	0
			2369	1562	395	392	20			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	expression tag	UNP P07700
A	32	GLY	-	expression tag	UNP P07700
A	68	SER	ARG	engineered mutation	UNP P07700
A	90	VAL	MET	engineered mutation	UNP P07700
A	116	LEU	CYS	engineered mutation	UNP P07700
A	227	ALA	TYR	engineered mutation	UNP P07700
A	?	-	CYS	deletion	UNP P07700
A	?	-	GLU	deletion	UNP P07700
A	?	-	GLY	deletion	UNP P07700
A	?	-	ARG	deletion	UNP P07700
A	?	-	PHE	deletion	UNP P07700
A	?	-	TYR	deletion	UNP P07700
A	?	-	GLY	deletion	UNP P07700
A	?	-	SER	deletion	UNP P07700
A	?	-	GLN	deletion	UNP P07700
A	?	-	GLU	deletion	UNP P07700
A	?	-	GLN	deletion	UNP P07700
A	?	-	PRO	deletion	UNP P07700
A	?	-	GLN	deletion	UNP P07700
A	?	-	PRO	deletion	UNP P07700
A	?	-	PRO	deletion	UNP P07700
A	?	-	PRO	deletion	UNP P07700
A	?	-	LEU	deletion	UNP P07700
A	?	-	PRO	deletion	UNP P07700
A	?	-	GLN	deletion	UNP P07700

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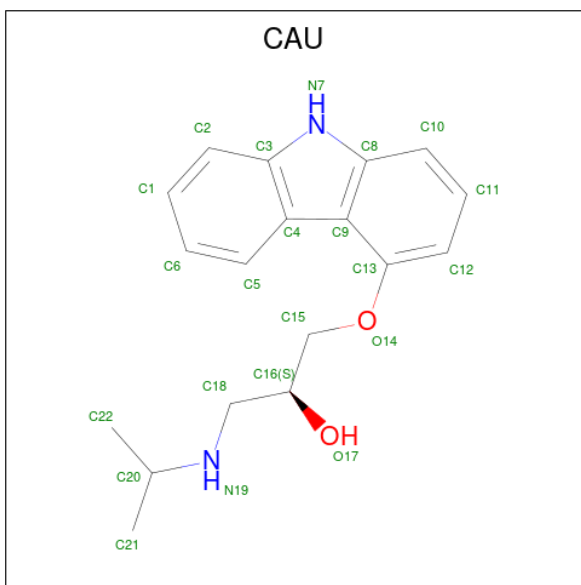
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	HIS	deletion	UNP P07700
A	?	-	GLN	deletion	UNP P07700
A	?	-	PRO	deletion	UNP P07700
A	?	-	ILE	deletion	UNP P07700
A	?	-	LEU	deletion	UNP P07700
A	?	-	GLY	deletion	UNP P07700
A	?	-	ASN	deletion	UNP P07700
A	?	-	GLY	deletion	UNP P07700
A	?	-	ARG	deletion	UNP P07700
A	?	-	THR	deletion	UNP P07700
A	?	-	SER	deletion	UNP P07700
A	282	LEU	ALA	engineered mutation	UNP P07700
A	327	ALA	PHE	engineered mutation	UNP P07700
A	338	MET	PHE	engineered mutation	UNP P07700
A	358	ALA	CYS	engineered mutation	UNP P07700
A	368	HIS	-	expression tag	UNP P07700
A	369	HIS	-	expression tag	UNP P07700
A	370	HIS	-	expression tag	UNP P07700
A	371	HIS	-	expression tag	UNP P07700
A	372	HIS	-	expression tag	UNP P07700
A	373	HIS	-	expression tag	UNP P07700
B	31	MET	-	expression tag	UNP P07700
B	32	GLY	-	expression tag	UNP P07700
B	68	SER	ARG	engineered mutation	UNP P07700
B	90	VAL	MET	engineered mutation	UNP P07700
B	116	LEU	CYS	engineered mutation	UNP P07700
B	227	ALA	TYR	engineered mutation	UNP P07700
B	?	-	CYS	deletion	UNP P07700
B	?	-	GLU	deletion	UNP P07700
B	?	-	GLY	deletion	UNP P07700
B	?	-	ARG	deletion	UNP P07700
B	?	-	PHE	deletion	UNP P07700
B	?	-	TYR	deletion	UNP P07700
B	?	-	GLY	deletion	UNP P07700
B	?	-	SER	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	GLU	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700

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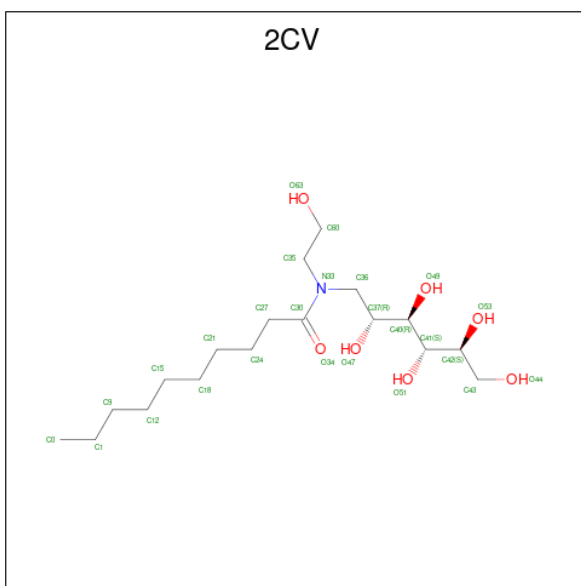
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P07700
B	?	-	LEU	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	HIS	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	ILE	deletion	UNP P07700
B	?	-	LEU	deletion	UNP P07700
B	?	-	GLY	deletion	UNP P07700
B	?	-	ASN	deletion	UNP P07700
B	?	-	GLY	deletion	UNP P07700
B	?	-	ARG	deletion	UNP P07700
B	?	-	THR	deletion	UNP P07700
B	?	-	SER	deletion	UNP P07700
B	282	LEU	ALA	engineered mutation	UNP P07700
B	327	ALA	PHE	engineered mutation	UNP P07700
B	338	MET	PHE	engineered mutation	UNP P07700
B	358	ALA	CYS	engineered mutation	UNP P07700
B	368	HIS	-	expression tag	UNP P07700
B	369	HIS	-	expression tag	UNP P07700
B	370	HIS	-	expression tag	UNP P07700
B	371	HIS	-	expression tag	UNP P07700
B	372	HIS	-	expression tag	UNP P07700
B	373	HIS	-	expression tag	UNP P07700

- Molecule 2 is (2S)-1-(9H-Carbazol-4-yloxy)-3-(isopropylamino)propan-2-ol (CCD ID: CAU) (formula: C₁₈H₂₂N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 22	C 18	N 2	O 2	0	0
2	B	1	Total 22	C 18	N 2	O 2	0	0

- Molecule 3 is HEGA-10 (CCD ID: 2CV) (formula: $\text{C}_{18}\text{H}_{37}\text{NO}_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 26	C 18	N 1	O 7	0	0
3	A	1	Total 26	C 18	N 1	O 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 26 18 1 7	0	0
3	B	1	Total C 10 10	0	0
3	B	1	Total C 10 10	0	0

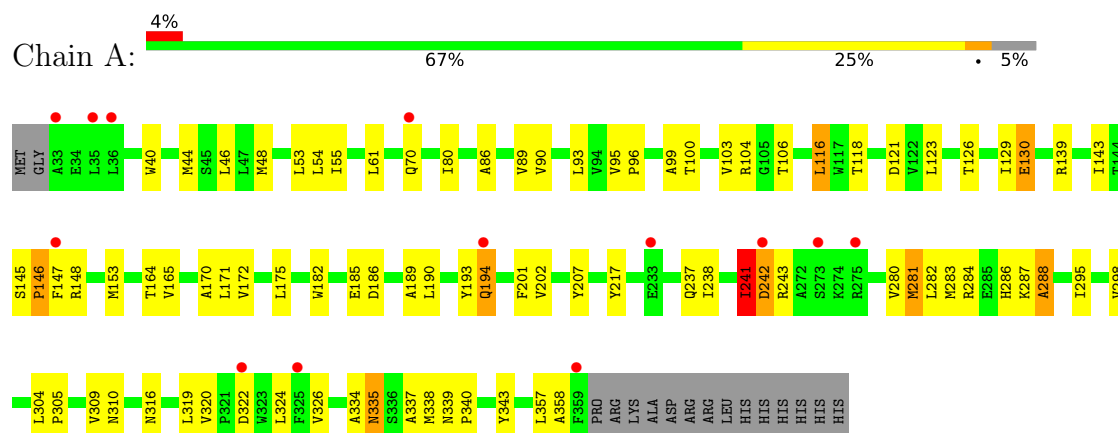
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

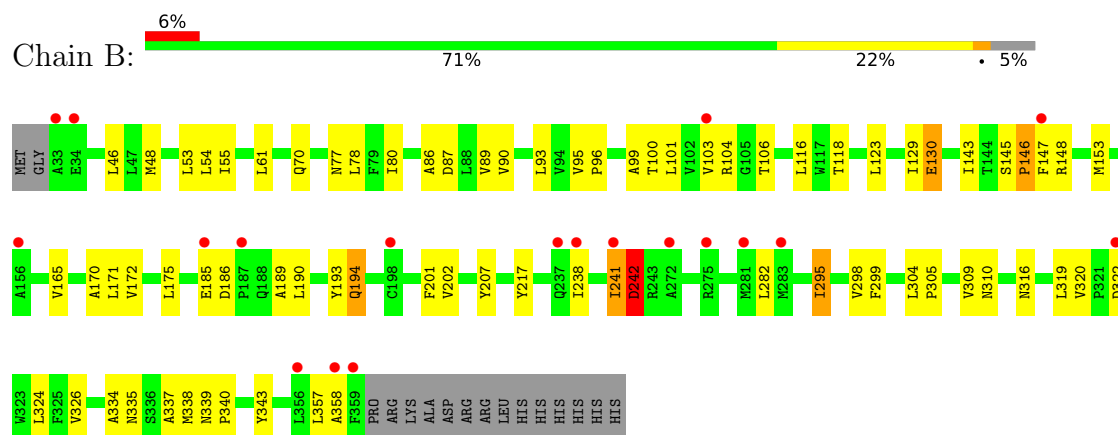
3 Residue-property plots

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: BETA-1 ADRENERGIC RECEPTOR



• Molecule 1: BETA-1 ADRENERGIC RECEPTOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.40Å 57.06Å 109.54Å 90.00° 113.52° 90.00°	Depositor
Resolution (Å)	44.68 – 3.00 44.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.68-3.00) 86.7 (44.68-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.248 , 0.295 0.248 , 0.295	Depositor DCC
R_{free} test set	913 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	74.3	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4882	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% 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: CAU, NA, 2CV

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	0.60	0/2425	0.85	3/3301 (0.1%)
1	B	0.61	0/2425	0.85	2/3301 (0.1%)
All	All	0.60	0/4850	0.85	5/6602 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ARG	N-CA-C	-9.28	101.17	111.28
1	B	148	ARG	N-CA-C	-7.86	102.71	111.28
1	A	241	ILE	N-CA-C	7.18	120.23	109.17
1	B	217	TYR	N-CA-C	5.58	117.36	111.28
1	A	217	TYR	N-CA-C	5.24	116.99	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	146	PRO	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	2369	0	2468	53	0
1	B	2369	0	2468	41	0
2	A	22	0	22	2	0
2	B	22	0	22	1	0
3	A	52	0	74	6	0
3	B	46	0	75	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	4882	0	5129	102	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 10.

All (102) 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:175:LEU:HD13	1:B:175:LEU:HD13	1.31	1.11
3:B:1360:2CV:O49	3:B:1360:2CV:H351	1.59	1.03
3:A:1361:2CV:H431	3:B:1362:2CV:H03C	1.41	1.01
1:B:171:LEU:HD12	1:B:175:LEU:HD12	1.48	0.95
1:A:171:LEU:HD12	1:A:175:LEU:HD12	1.47	0.94
1:B:241:ILE:HD11	1:B:282:LEU:HD12	1.51	0.92
1:A:89:VAL:HG13	1:A:93:LEU:HD12	1.67	0.76
1:A:171:LEU:HD12	1:A:175:LEU:CD1	2.16	0.74
1:B:171:LEU:HD12	1:B:175:LEU:CD1	2.18	0.73
1:A:287:LYS:O	1:A:288:ALA:CB	2.38	0.72
1:A:241:ILE:HG23	1:A:242:ASP:N	2.07	0.69
1:B:89:VAL:HG13	1:B:93:LEU:HD12	1.73	0.68
3:A:1361:2CV:H431	3:B:1362:2CV:C0	2.22	0.66
1:B:241:ILE:HG22	1:B:242:ASP:N	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ILE:CG1	1:B:337:ALA:HB2	2.27	0.65
1:B:118:THR:HG21	1:B:201:PHE:CE1	2.32	0.65
1:B:55:ILE:HG13	1:B:337:ALA:HB2	1.81	0.63
1:A:55:ILE:CG1	1:A:337:ALA:HB2	2.29	0.61
1:A:118:THR:HG21	1:A:201:PHE:CE1	2.35	0.61
1:A:287:LYS:O	1:A:288:ALA:HB3	2.00	0.61
1:A:241:ILE:HG23	1:A:242:ASP:H	1.67	0.60
1:B:320:VAL:HG13	1:B:324:LEU:HD23	1.84	0.59
1:A:189:ALA:HB1	1:A:193:TYR:CZ	2.39	0.58
1:A:116:LEU:HD12	1:A:116:LEU:O	2.04	0.57
1:B:116:LEU:HD12	1:B:116:LEU:O	2.04	0.57
1:B:86:ALA:O	1:B:90:VAL:HG23	2.04	0.57
1:A:55:ILE:HG13	1:A:337:ALA:HB2	1.86	0.56
1:B:320:VAL:CG1	1:B:324:LEU:HD23	2.35	0.56
1:A:320:VAL:HG13	1:A:324:LEU:HD23	1.88	0.56
1:B:316:ASN:ND2	1:B:319:LEU:HD22	2.21	0.55
1:A:130:GLU:HB3	1:A:165:VAL:HG13	1.90	0.54
1:A:237:GLN:HE22	1:A:282:LEU:HD22	1.73	0.54
1:A:241:ILE:CG2	1:A:242:ASP:N	2.71	0.54
1:A:339:ASN:HB2	1:A:340:PRO:HD3	1.90	0.54
1:A:237:GLN:OE1	1:A:286:HIS:NE2	2.37	0.53
1:B:130:GLU:HB3	1:B:165:VAL:HG13	1.91	0.53
1:A:164:THR:HG23	3:B:1360:2CV:H431	1.91	0.53
1:A:118:THR:HG21	1:A:201:PHE:CD1	2.43	0.52
1:B:339:ASN:HB2	1:B:340:PRO:HD3	1.90	0.52
1:B:335:ASN:N	1:B:338:MET:HE3	2.23	0.52
1:A:320:VAL:CG1	1:A:324:LEU:HD23	2.40	0.52
1:A:319:LEU:HD12	1:A:319:LEU:O	2.10	0.52
1:A:121:ASP:OD1	2:A:400:CAU:O17	2.20	0.51
1:B:95:VAL:O	1:B:99:ALA:N	2.36	0.51
1:B:103:VAL:HG12	1:B:104:ARG:N	2.25	0.51
1:A:96:PRO:O	1:A:100:THR:HG23	2.11	0.51
1:A:310:ASN:HD21	2:A:400:CAU:C6	2.24	0.51
1:B:55:ILE:HG12	1:B:337:ALA:HB2	1.93	0.51
1:A:55:ILE:HG12	1:A:337:ALA:HB2	1.92	0.50
1:A:95:VAL:O	1:A:96:PRO:C	2.55	0.50
1:A:316:ASN:ND2	1:A:319:LEU:HD22	2.26	0.50
1:B:118:THR:HG21	1:B:201:PHE:CD1	2.46	0.50
1:B:319:LEU:O	1:B:319:LEU:HD12	2.11	0.50
1:A:280:VAL:HG12	1:A:280:VAL:O	2.12	0.50
1:A:322:ASP:O	1:A:326:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ALA:C	1:A:338:MET:HE3	2.37	0.49
1:B:189:ALA:HB1	1:B:193:TYR:CZ	2.47	0.48
1:A:89:VAL:HG13	1:A:93:LEU:CD1	2.40	0.48
3:A:1360:2CV:H40	3:A:1360:2CV:H432	1.56	0.48
1:B:96:PRO:O	1:B:100:THR:HG23	2.14	0.48
1:B:207:TYR:CD1	1:B:207:TYR:C	2.93	0.47
3:B:1360:2CV:H272	3:B:1360:2CV:H361	1.65	0.47
1:A:103:VAL:HG12	1:A:104:ARG:N	2.29	0.47
1:B:129:ILE:HD13	1:B:299:PHE:CE1	2.50	0.47
1:B:334:ALA:C	1:B:338:MET:HE3	2.39	0.47
1:B:80:ILE:HG23	1:B:343:TYR:OH	2.16	0.46
3:A:1361:2CV:O47	3:A:1361:2CV:H271	2.15	0.45
1:B:322:ASP:O	1:B:326:VAL:HG23	2.16	0.45
1:A:86:ALA:O	1:A:90:VAL:HG23	2.17	0.45
1:B:357:LEU:O	1:B:358:ALA:HB3	2.17	0.44
3:B:1360:2CV:H351	3:B:1360:2CV:H49	1.76	0.44
1:A:189:ALA:HB1	1:A:193:TYR:OH	2.16	0.44
1:B:310:ASN:HD21	2:B:400:CAU:C6	2.29	0.44
1:A:207:TYR:CD1	1:A:207:TYR:C	2.96	0.44
1:A:304:LEU:N	1:A:305:PRO:CD	2.80	0.44
1:A:238:ILE:HG13	1:A:241:ILE:HD12	1.99	0.44
1:B:304:LEU:N	1:B:305:PRO:CD	2.81	0.44
1:B:190:LEU:O	1:B:194:GLN:HG2	2.17	0.43
1:A:190:LEU:O	1:A:194:GLN:HG2	2.18	0.43
1:B:238:ILE:HG13	1:B:241:ILE:HD12	2.01	0.43
1:A:95:VAL:O	1:A:99:ALA:N	2.38	0.43
1:A:335:ASN:N	1:A:338:MET:HE3	2.33	0.43
1:A:357:LEU:O	1:A:358:ALA:HB3	2.19	0.42
1:B:89:VAL:HG13	1:B:93:LEU:CD1	2.46	0.42
1:B:99:ALA:C	1:B:101:LEU:H	2.28	0.42
1:A:182:TRP:CD1	1:A:182:TRP:H	2.38	0.42
1:A:281:MET:HE2	1:A:281:MET:HB2	1.93	0.42
1:B:87:ASP:O	1:B:90:VAL:HB	2.20	0.42
1:B:46:LEU:HD12	1:B:46:LEU:HA	1.94	0.41
3:A:1360:2CV:H271	3:A:1360:2CV:H352	1.77	0.41
1:A:126:THR:O	1:A:129:ILE:HG22	2.21	0.41
1:B:295:ILE:CD1	1:B:339:ASN:OD1	2.68	0.41
3:A:1361:2CV:C24	3:A:1361:2CV:H362	2.51	0.41
1:A:241:ILE:C	1:A:243:ARG:H	2.28	0.41
1:A:80:ILE:HD12	1:A:343:TYR:OH	2.21	0.41
1:A:139:ARG:HA	1:A:139:ARG:NE	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:TRP:CZ2	1:A:44:MET:HE3	2.55	0.41
1:A:123:LEU:HD13	1:A:170:ALA:HA	2.03	0.41
1:B:77:ASN:HA	1:B:80:ILE:HB	2.03	0.40
1:A:80:ILE:HG23	1:A:343:TYR:OH	2.20	0.40
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.91	0.40
1:B:123:LEU:HD13	1:B:170:ALA:HA	2.03	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	295/313 (94%)	265 (90%)	27 (9%)	3 (1%)	12	45
1	B	295/313 (94%)	268 (91%)	25 (8%)	2 (1%)	18	53
All	All	590/626 (94%)	533 (90%)	52 (9%)	5 (1%)	16	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	242	ASP
1	A	242	ASP
1	A	288	ALA
1	A	146	PRO
1	B	146	PRO

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	257/271 (95%)	232 (90%)	25 (10%)	8	30
1	B	257/271 (95%)	235 (91%)	22 (9%)	10	36
All	All	514/542 (95%)	467 (91%)	47 (9%)	9	33

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	MET
1	A	53	LEU
1	A	54	LEU
1	A	61	LEU
1	A	70	GLN
1	A	106	THR
1	A	116	LEU
1	A	130	GLU
1	A	143	ILE
1	A	145	SER
1	A	147	PHE
1	A	153	MET
1	A	172	VAL
1	A	185	GLU
1	A	186	ASP
1	A	194	GLN
1	A	202	VAL
1	A	241	ILE
1	A	281	MET
1	A	283	MET
1	A	284	ARG
1	A	295	ILE
1	A	298	VAL
1	A	309	VAL
1	A	335	ASN
1	B	48	MET
1	B	53	LEU
1	B	54	LEU
1	B	61	LEU
1	B	70	GLN
1	B	78	LEU
1	B	106	THR
1	B	130	GLU

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Mol	Chain	Res	Type
1	B	143	ILE
1	B	145	SER
1	B	147	PHE
1	B	153	MET
1	B	172	VAL
1	B	185	GLU
1	B	186	ASP
1	B	194	GLN
1	B	202	VAL
1	B	241	ILE
1	B	242	ASP
1	B	295	ILE
1	B	298	VAL
1	B	309	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	310	ASN
1	A	316	ASN
1	B	310	ASN

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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	CAU	A	400	-	24,24,24	1.32	4 (16%)	33,33,33	1.30	4 (12%)
2	CAU	B	400	-	24,24,24	1.45	4 (16%)	33,33,33	1.30	5 (15%)
3	2CV	B	1362	-	9,9,25	0.62	0	8,8,30	0.39	0
3	2CV	A	1360	-	25,25,25	0.77	0	29,30,30	0.72	0
3	2CV	B	1360	-	25,25,25	0.92	2 (8%)	29,30,30	1.12	1 (3%)
3	2CV	A	1361	-	25,25,25	0.67	0	29,30,30	0.58	0
3	2CV	B	1361	-	9,9,25	0.66	0	8,8,30	0.38	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
2	CAU	A	400	-	-	2/10/10/10	0/3/3/3
2	CAU	B	400	-	-	0/10/10/10	0/3/3/3
3	2CV	B	1362	-	-	1/7/7/34	-
3	2CV	A	1360	-	-	13/34/34/34	-
3	2CV	B	1360	-	-	17/34/34/34	-
3	2CV	A	1361	-	-	21/34/34/34	-
3	2CV	B	1361	-	-	4/7/7/34	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	CAU	C4-C9	-3.91	1.37	1.46
2	A	400	CAU	C4-C9	-3.42	1.38	1.46
2	A	400	CAU	C8-N7	-3.04	1.33	1.38
2	B	400	CAU	C8-N7	-3.03	1.33	1.38
2	A	400	CAU	C3-N7	-2.98	1.33	1.38
2	B	400	CAU	C3-N7	-2.90	1.33	1.38
2	B	400	CAU	C9-C8	-2.86	1.38	1.41
3	B	1360	2CV	C36-C37	2.42	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	CAU	C9-C8	-2.38	1.38	1.41
3	B	1360	2CV	C42-C41	2.35	1.57	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1360	2CV	C35-N33-C36	3.83	120.48	116.14
2	A	400	CAU	C18-N19-C20	-3.51	103.62	114.38
2	B	400	CAU	C18-N19-C20	-3.18	104.64	114.38
2	B	400	CAU	C8-C9-C13	3.07	121.59	118.64
2	A	400	CAU	O14-C13-C9	2.62	119.65	115.52
2	B	400	CAU	C2-C3-C4	-2.47	119.11	121.68
2	A	400	CAU	C8-C9-C13	2.38	120.92	118.64
2	B	400	CAU	C10-C8-C9	-2.33	119.56	122.37
2	B	400	CAU	C2-C3-N7	2.24	132.26	129.07
2	A	400	CAU	C15-O14-C13	-2.14	113.47	118.21

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1360	2CV	N33-C36-C37-C40
3	A	1360	2CV	N33-C36-C37-O47
3	A	1360	2CV	C40-C41-C42-C43
3	A	1360	2CV	C40-C41-C42-O53
3	A	1360	2CV	O51-C41-C42-O53
3	A	1360	2CV	O53-C42-C43-O44
3	A	1361	2CV	C37-C40-C41-C42
3	A	1361	2CV	O49-C40-C41-C42
3	A	1361	2CV	C40-C41-C42-O53
3	A	1361	2CV	O51-C41-C42-O53
3	A	1361	2CV	C41-C42-C43-O44
3	A	1361	2CV	O53-C42-C43-O44
3	B	1360	2CV	C37-C36-N33-C35
3	B	1360	2CV	N33-C36-C37-C40
3	A	1361	2CV	N33-C35-C60-O63
3	A	1360	2CV	C41-C42-C43-O44
3	A	1361	2CV	O51-C41-C42-C43
3	A	1361	2CV	C40-C41-C42-C43
3	A	1361	2CV	O49-C40-C41-O51
3	A	1361	2CV	C21-C24-C27-C30
3	B	1360	2CV	O51-C41-C42-C43

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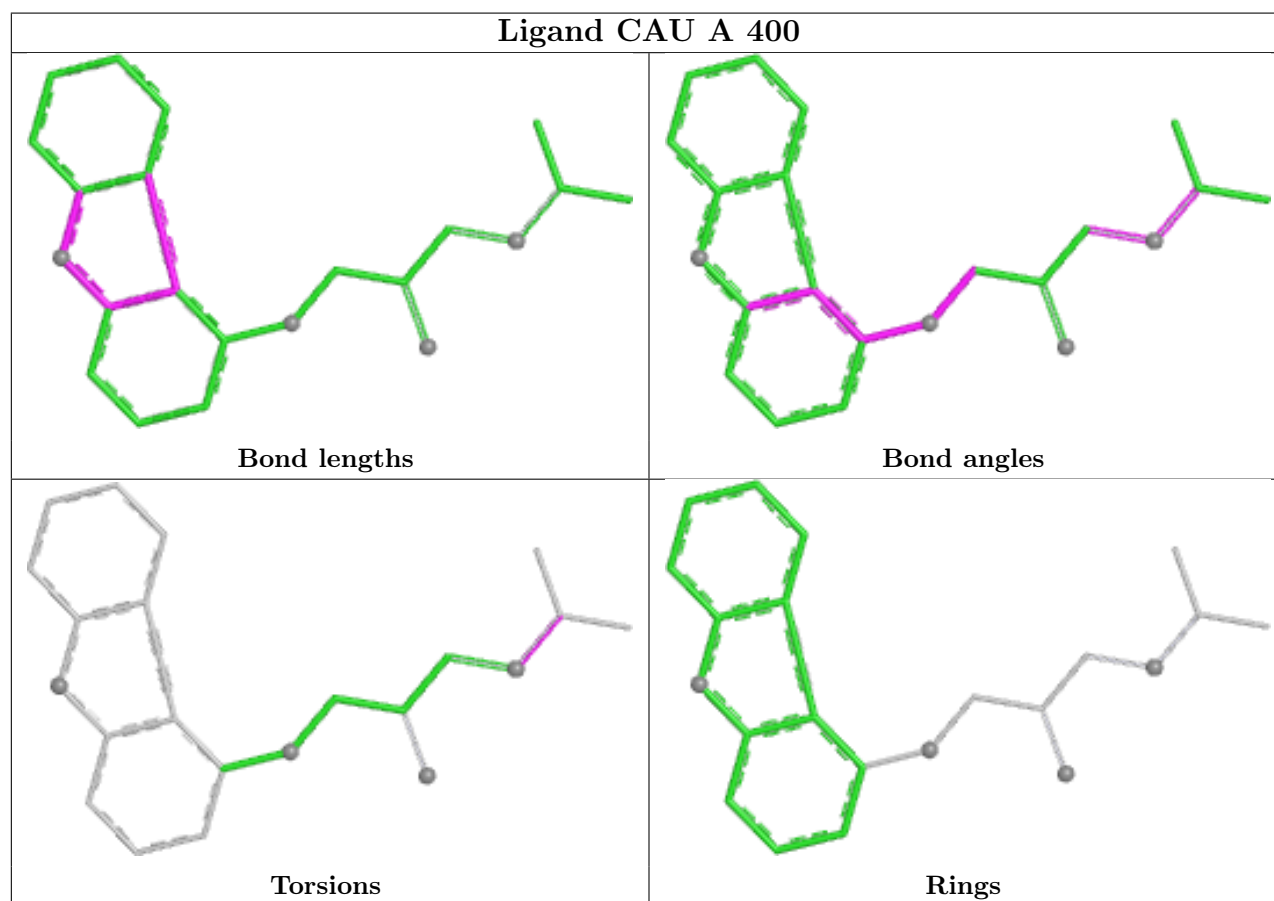
Mol	Chain	Res	Type	Atoms
3	B	1360	2CV	C37-C36-N33-C30
3	A	1361	2CV	C37-C40-C41-O51
3	A	1360	2CV	O49-C40-C41-C42
3	B	1360	2CV	C40-C41-C42-O53
3	B	1360	2CV	N33-C35-C60-O63
3	A	1360	2CV	O51-C41-C42-C43
3	B	1360	2CV	C18-C21-C24-C27
3	A	1360	2CV	C37-C40-C41-C42
3	B	1360	2CV	O49-C40-C41-O51
3	A	1361	2CV	C15-C18-C21-C24
3	B	1360	2CV	O53-C42-C43-O44
2	A	400	CAU	C21-C20-N19-C18
2	A	400	CAU	C22-C20-N19-C18
3	B	1360	2CV	O51-C41-C42-O53
3	A	1361	2CV	C12-C15-C18-C21
3	B	1360	2CV	C40-C41-C42-C43
3	B	1360	2CV	C9-C12-C15-C18
3	B	1361	2CV	C0-C1-C9-C12
3	A	1361	2CV	C0-C1-C9-C12
3	A	1361	2CV	C15-C12-C9-C1
3	B	1360	2CV	C37-C40-C41-O51
3	A	1361	2CV	C60-C35-N33-C30
3	B	1360	2CV	O47-C37-C40-C41
3	A	1360	2CV	C15-C18-C21-C24
3	B	1360	2CV	C15-C12-C9-C1
3	B	1361	2CV	C9-C12-C15-C18
3	A	1361	2CV	C9-C12-C15-C18
3	B	1362	2CV	C15-C12-C9-C1
3	B	1360	2CV	O47-C37-C40-O49
3	A	1361	2CV	C24-C27-C30-O34
3	A	1360	2CV	C18-C21-C24-C27
3	B	1361	2CV	C15-C18-C21-C24
3	A	1361	2CV	O47-C37-C40-C41
3	B	1361	2CV	C15-C12-C9-C1
3	B	1360	2CV	C15-C18-C21-C24
3	A	1361	2CV	C24-C27-C30-N33
3	A	1360	2CV	C12-C15-C18-C21

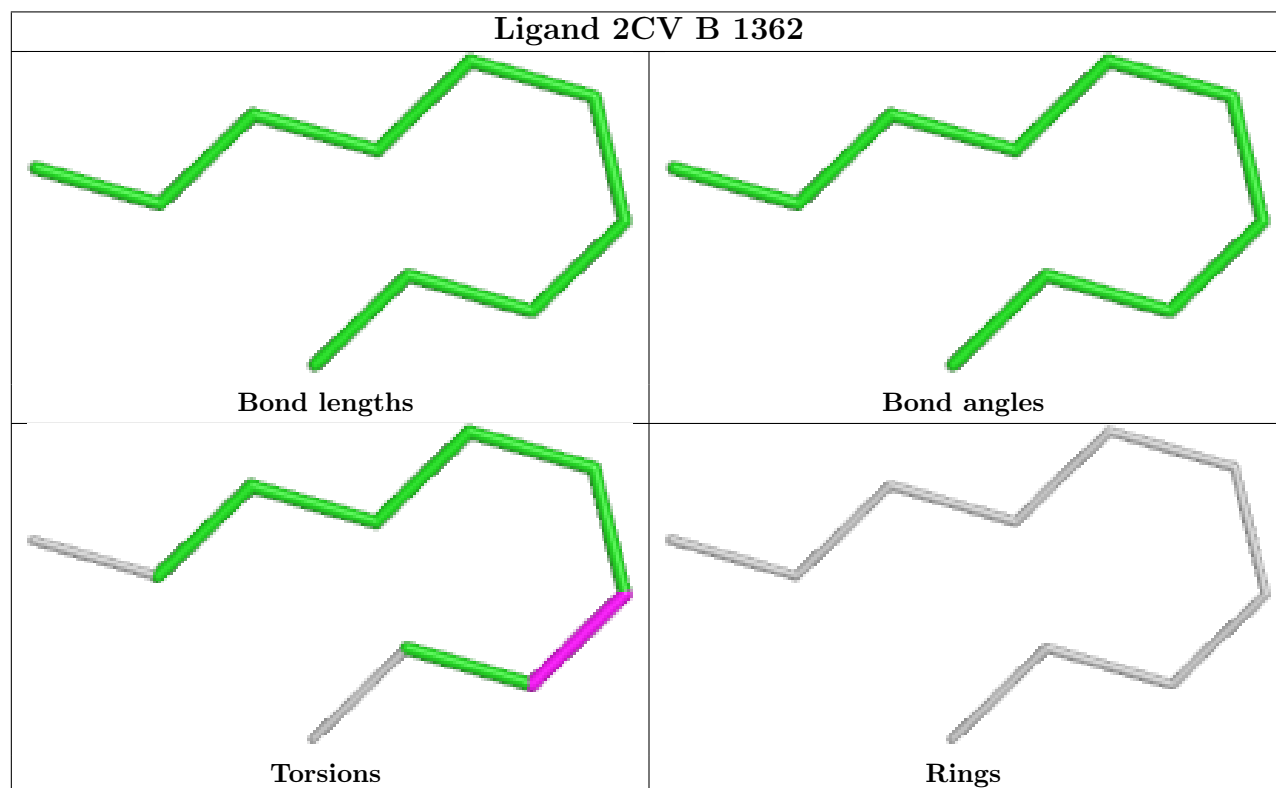
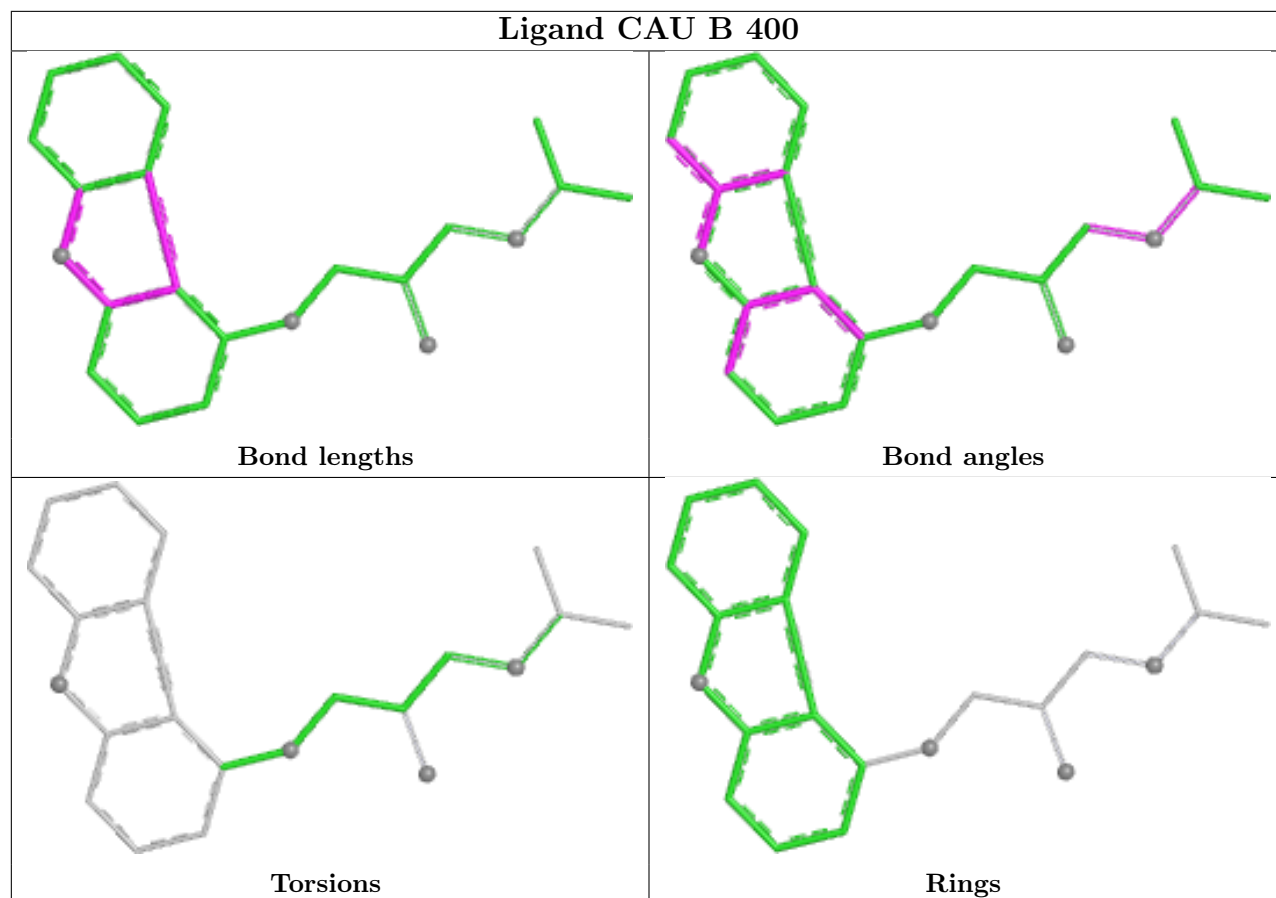
There are no ring outliers.

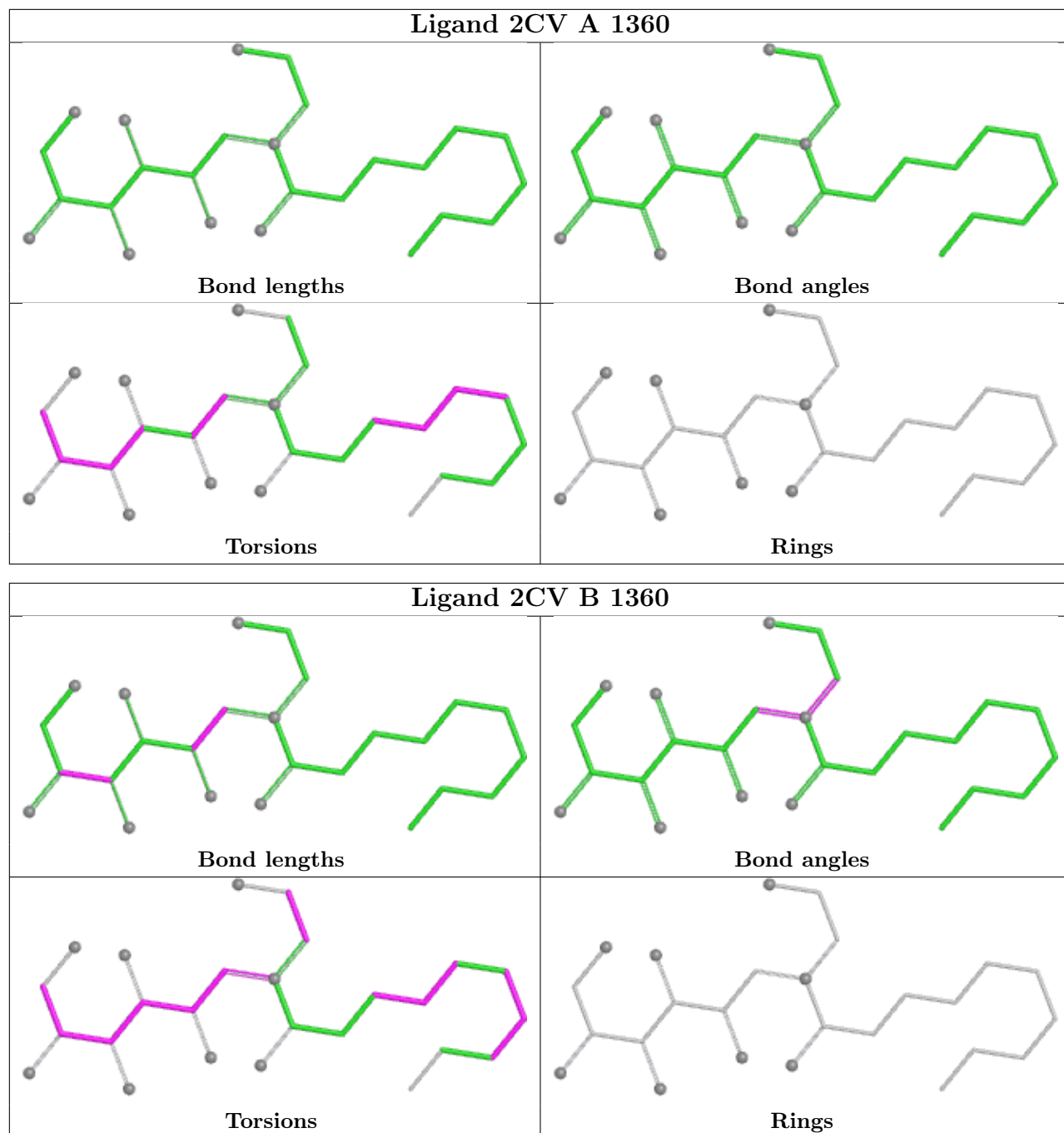
6 monomers are involved in 13 short contacts:

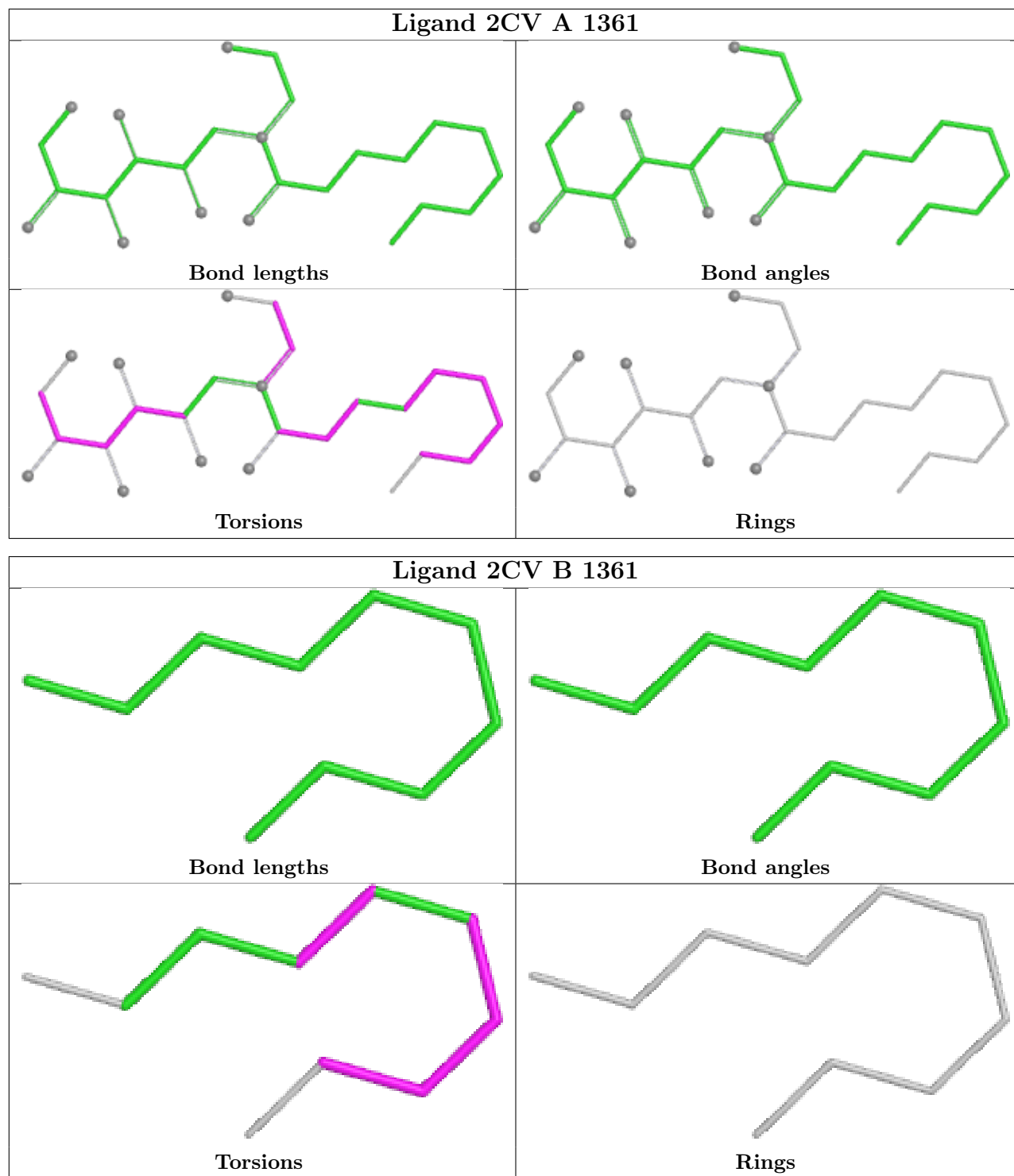
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	CAU	2	0
2	B	400	CAU	1	0
3	B	1362	2CV	2	0
3	A	1360	2CV	2	0
3	B	1360	2CV	4	0
3	A	1361	2CV	4	0

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

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	297/313 (94%)	0.29	13 (4%) 39 21	34, 61, 102, 137	0
1	B	297/313 (94%)	0.39	19 (6%) 25 13	34, 61, 112, 138	0
All	All	594/626 (94%)	0.34	32 (5%) 31 16	34, 61, 105, 138	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	238	ILE	4.1
1	B	359	PHE	3.9
1	B	322	ASP	3.7
1	A	147	PHE	3.6
1	A	36	LEU	3.3
1	B	241	ILE	3.3
1	A	194	GLN	3.2
1	A	322	ASP	3.2
1	B	147	PHE	3.1
1	B	358	ALA	3.1
1	A	325	PHE	2.9
1	B	283	MET	2.9
1	A	359	PHE	2.9
1	B	187	PRO	2.6
1	A	273	SER	2.5
1	B	34	GLU	2.5
1	A	35	LEU	2.5
1	A	233	GLU	2.5
1	B	272	ALA	2.4
1	B	185	GLU	2.4
1	B	103	VAL	2.4
1	A	242	ASP	2.4
1	A	33	ALA	2.3
1	B	198	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	281	MET	2.3
1	B	237	GLN	2.3
1	B	275	ARG	2.3
1	B	156	ALA	2.3
1	A	70	GLN	2.2
1	B	33	ALA	2.2
1	B	356	LEU	2.2
1	A	275	ARG	2.1

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

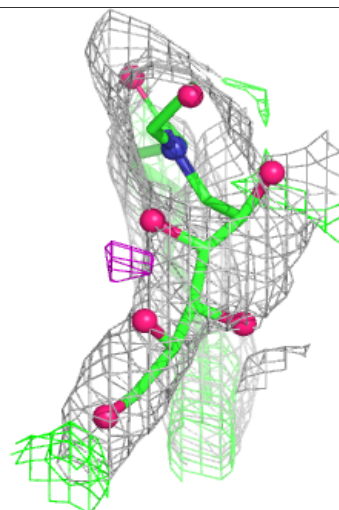
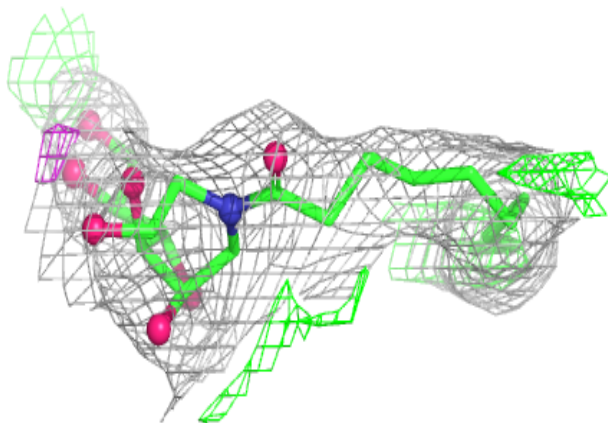
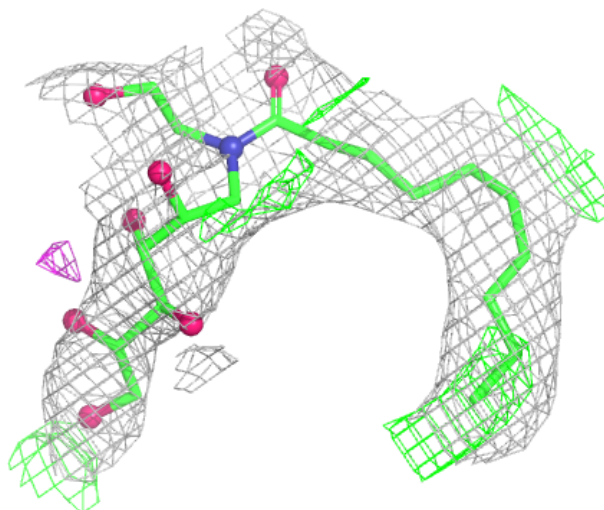
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	2CV	B	1360	26/26	0.81	0.21	67,78,84,85	0
3	2CV	B	1361	10/26	0.81	0.27	63,65,66,66	0
3	2CV	A	1360	26/26	0.84	0.17	91,110,112,113	0
4	NA	A	1362	1/1	0.84	0.12	64,64,64,64	0
4	NA	B	1363	1/1	0.86	0.11	67,67,67,67	0
3	2CV	A	1361	26/26	0.88	0.15	62,78,81,82	0
3	2CV	B	1362	10/26	0.88	0.21	75,77,77,77	0
2	CAU	A	400	22/22	0.95	0.10	48,53,54,54	0
2	CAU	B	400	22/22	0.96	0.10	48,50,51,52	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.

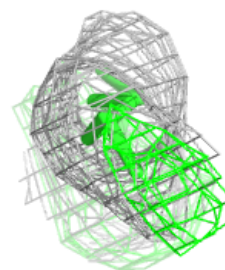
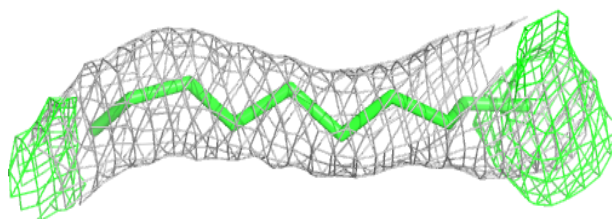
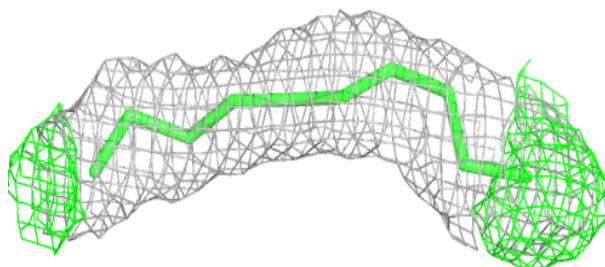
Electron density around 2CV B 1360:

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

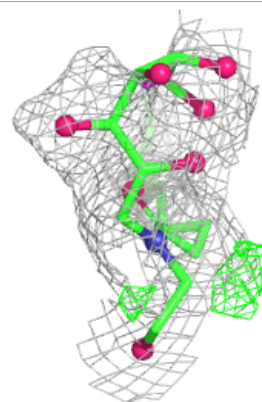
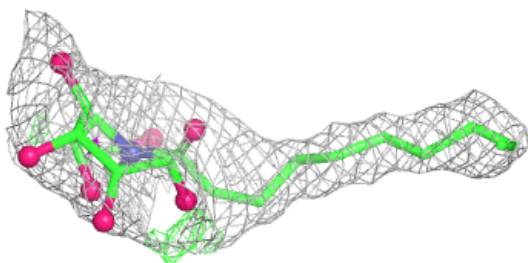
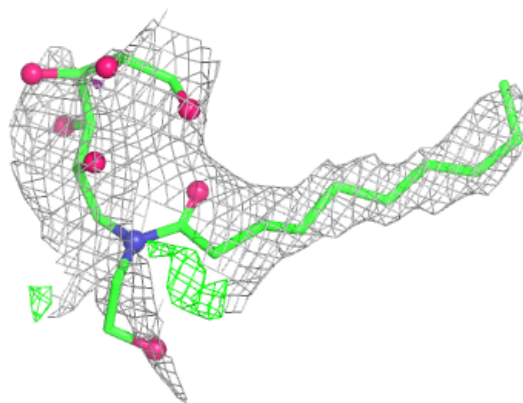


Electron density around 2CV B 1361:

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

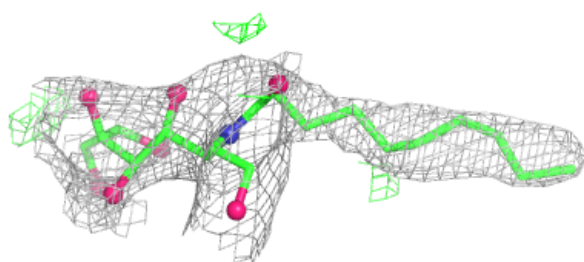
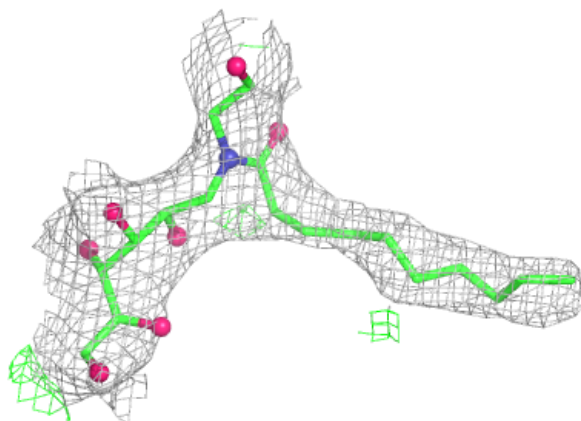
**Electron density around 2CV A 1360:**

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

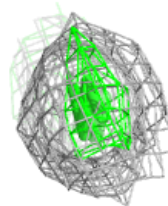
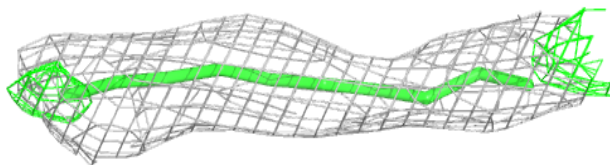
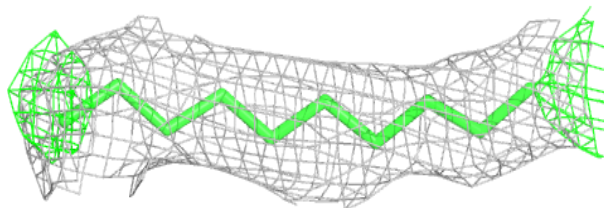


Electron density around 2CV A 1361:

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

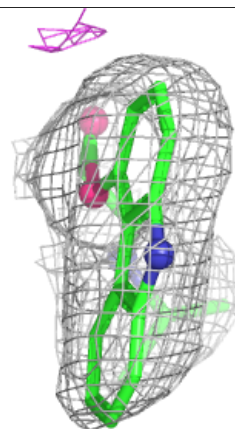
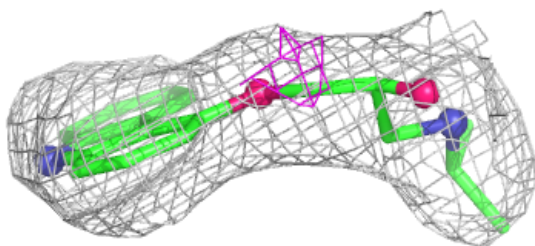
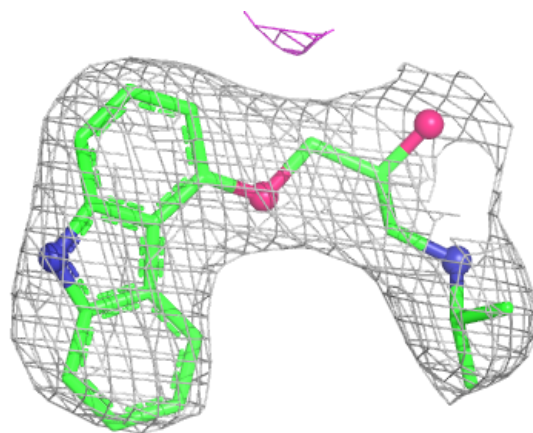
**Electron density around 2CV B 1362:**

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

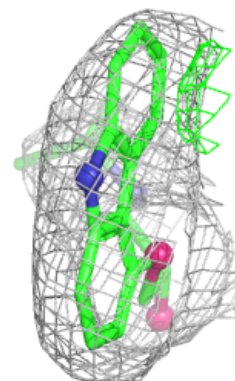
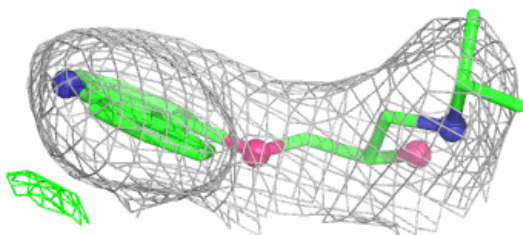
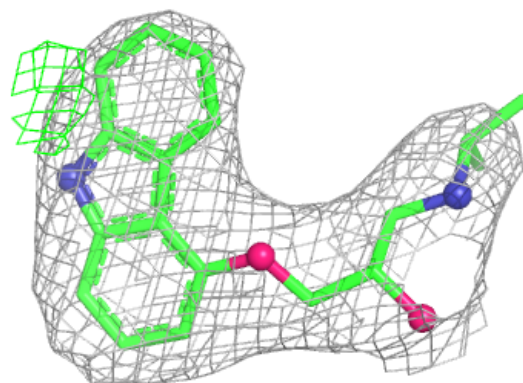


Electron density around CAU A 400:

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

**Electron density around CAU B 400:**

$2mF_o-DF_c$ (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.