



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:30 PM UTC

PDB ID : 6IBL / pdb_00006ibl
Title : ACTIVATED TURKEY BETA1 ADRENOCEPTOR WITH BOUND AGONIST FORMOTEROL AND NANOBODY Nb80
Authors : Warne, T.; Edwards, P.C.; Dore, A.S.; Leslie, A.G.W.; Tate, C.G.
Deposited on : 2018-11-30
Resolution : 2.70 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

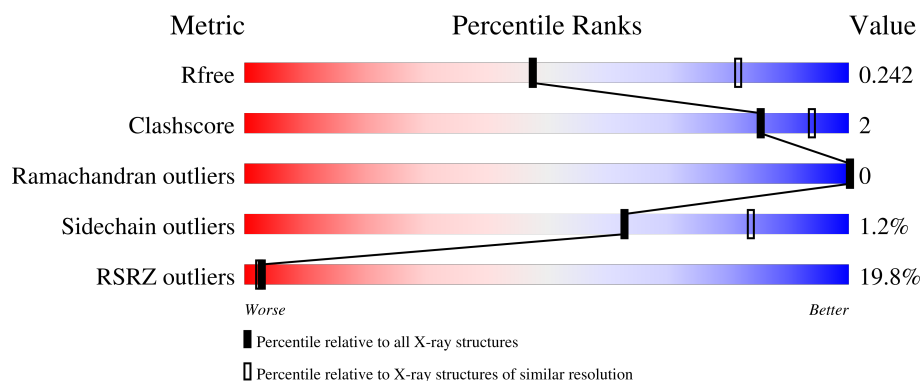
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	416	19% 90% 6% 5%
1	B	416	23% 88% 6% 6%
2	C	121	9% 88% 11% .
2	D	121	12% 90% 9% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8271 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 Thioredoxin 1, Beta-1 adrenergic receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3105	2036	512	537	20			
1	B	391	Total	C	N	O	S	0	0	0
			3068	2017	501	531	19			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1032	SER	CYS	engineered mutation	UNP P0AA25
A	1035	SER	CYS	engineered mutation	UNP P0AA25
A	1109	GLU	-	linker	UNP P0AA25
A	39	ALA	-	linker	UNP P0AA25
A	40	ALA	-	linker	UNP P0AA25
A	41	ALA	-	linker	UNP P0AA25
A	42	LYS	-	linker	UNP P0AA25
A	43	VAL	-	linker	UNP P0AA25
A	68	SER	ARG	conflict	UNP P07700
A	90	VAL	MET	conflict	UNP P07700
A	116	LEU	CYS	conflict	UNP P07700
A	?	-	ARG	deletion	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	284	LYS	ARG	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	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	1032	SER	CYS	engineered mutation	UNP P0AA25
B	1035	SER	CYS	engineered mutation	UNP P0AA25
B	1109	GLU	-	linker	UNP P0AA25
B	39	ALA	-	linker	UNP P0AA25
B	40	ALA	-	linker	UNP P0AA25
B	41	ALA	-	linker	UNP P0AA25
B	42	LYS	-	linker	UNP P0AA25
B	43	VAL	-	linker	UNP P0AA25
B	68	SER	ARG	conflict	UNP P07700
B	90	VAL	MET	conflict	UNP P07700
B	116	LEU	CYS	conflict	UNP P07700
B	?	-	ARG	deletion	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

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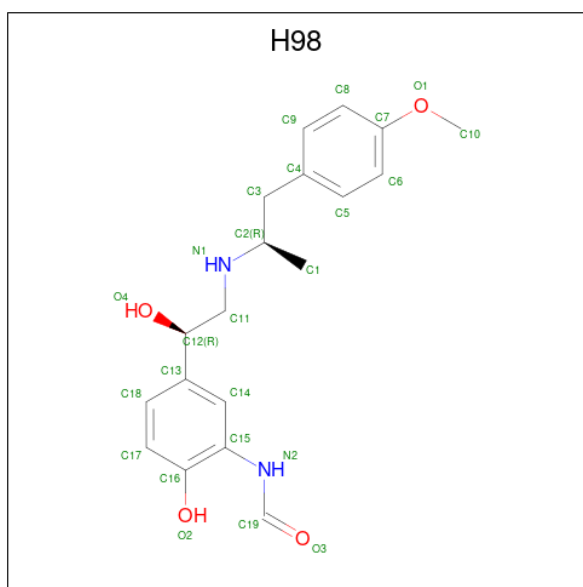
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	GLU	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
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	284	LYS	ARG	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	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 a protein called Camelid antibody fragment Nb80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	119	Total	C	N	O	S	0	0	0
			901	561	157	179	4			
2	D	120	Total	C	N	O	S	0	0	0
			910	566	159	181	4			

- Molecule 3 is {N}-[5-[(1 {R})-2-[(2 {R})-1-(4-methoxyphenyl)propan-2-yl]amino]-1-oxidan-yl-ethyl]-2-oxidanyl-phenyl]methanamide (CCD ID: H98) (formula: C₁₉H₂₄N₂O₄).

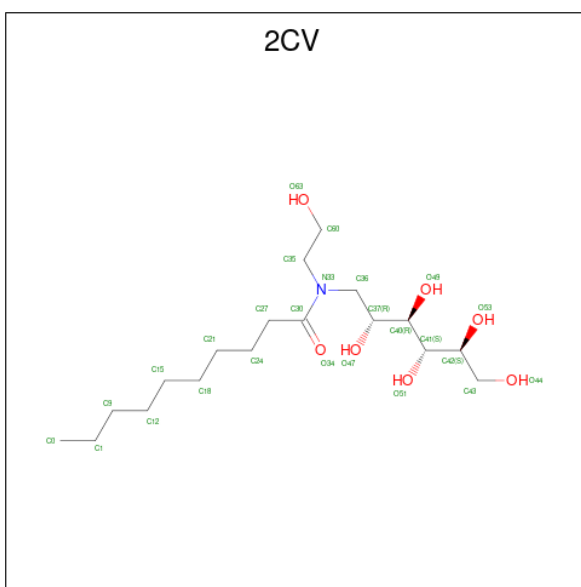


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	19	2	4		
3	B	1	Total	C	N	O	0	0
			25	19	2	4		

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

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

- Molecule 5 is HEGA-10 (CCD ID: 2CV) (formula: C₁₈H₃₇NO₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 26	C 18	N 1	O 7	0	0
5	A	1	Total 26	C 18	N 1	O 7	0	0
5	A	1	Total 24	C 16	N 1	O 7	0	0
5	A	1	Total 26	C 18	N 1	O 7	0	0
5	A	1	Total 26	C 18	N 1	O 7	0	0
5	B	1	Total 26	C 18	N 1	O 7	0	0
5	B	1	Total 26	C 18	N 1	O 7	0	0
5	B	1	Total 26	C 18	N 1	O 7	0	0

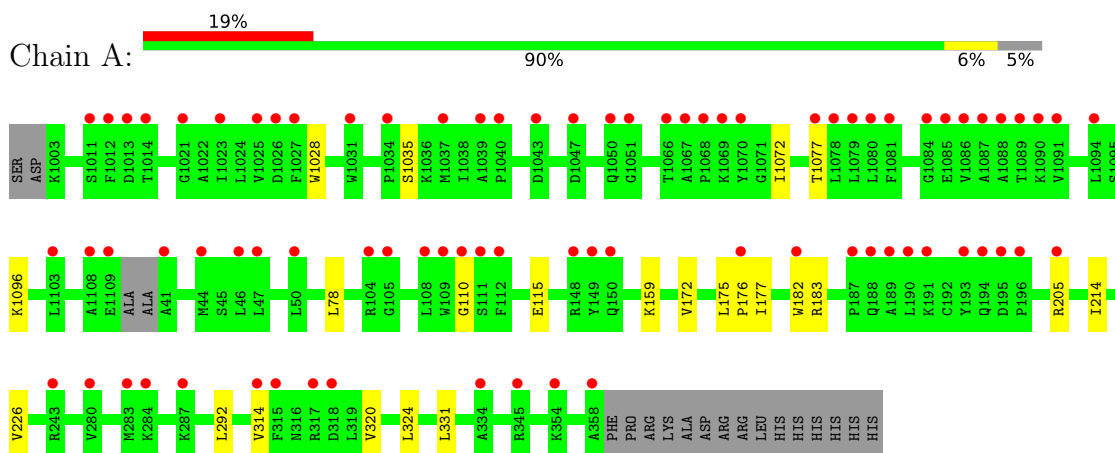
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O 8 8	0	0
6	C	6	Total O 6 6	0	0
6	B	11	Total O 11 11	0	0
6	D	4	Total O 4 4	0	0

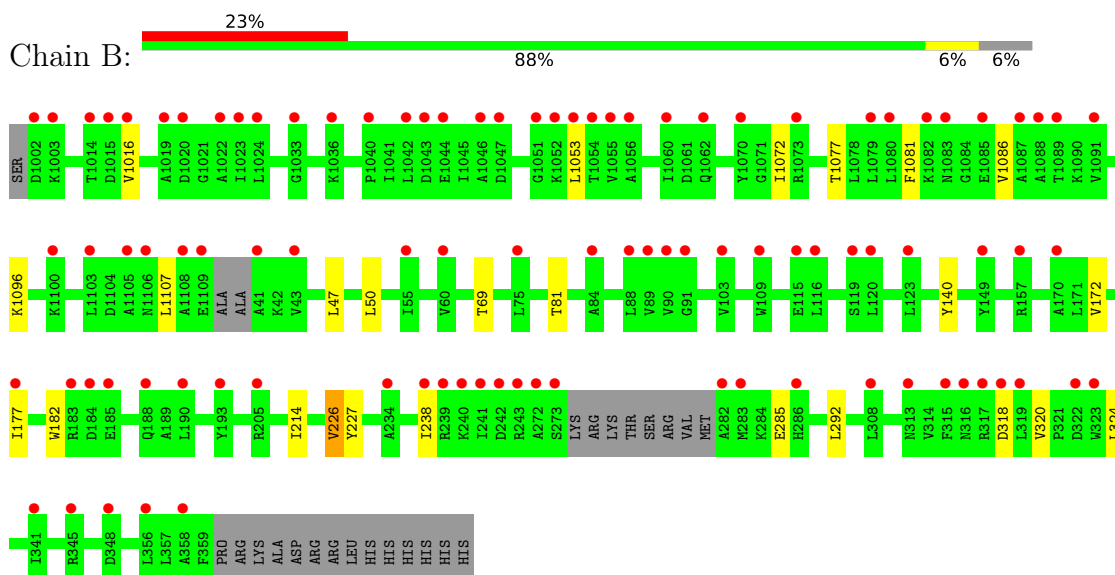
3 Residue-property plots

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.

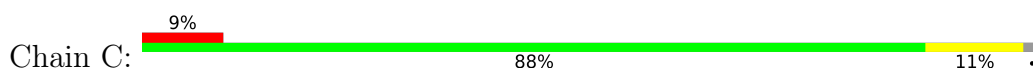
- Molecule 1: Thioredoxin 1, Beta-1 adrenergic receptor

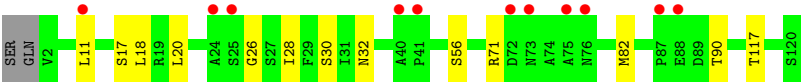


- Molecule 1: Thioredoxin 1, Beta-1 adrenergic receptor

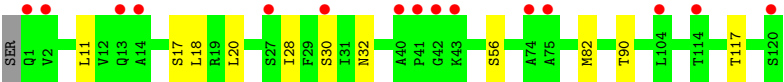
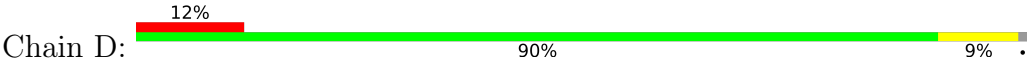


- Molecule 2: Camelid antibody fragment Nb80





● Molecule 2: Camelid antibody fragment Nb80



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.65Å 121.12Å 129.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.32 – 2.70 44.32 – 2.71	Depositor EDS
% Data completeness (in resolution range)	62.7 (44.32-2.70) 62.7 (44.32-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.35 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.240 , 0.277 0.244 , 0.242	Depositor DCC
R_{free} test set	2558 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 23.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.031 for k,h,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8271	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: 2CV, NA, H98

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	1.13	0/3174	1.70	6/4322 (0.1%)
1	B	1.11	0/3137	1.68	4/4270 (0.1%)
2	C	1.07	0/918	1.41	1/1244 (0.1%)
2	D	1.08	0/927	1.45	0/1256
All	All	1.11	0/8156	1.63	11/11092 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1096	LYS	CA-C-N	5.92	126.55	119.98
1	B	1096	LYS	C-N-CA	5.92	126.55	119.98
1	B	69	THR	CA-C-N	5.49	127.63	120.28
1	B	69	THR	C-N-CA	5.49	127.63	120.28
1	A	110	GLY	CA-C-N	5.28	128.74	120.82
1	A	110	GLY	C-N-CA	5.28	128.74	120.82
1	A	1096	LYS	CA-C-N	5.21	125.76	119.98
1	A	1096	LYS	C-N-CA	5.21	125.76	119.98
1	A	331	LEU	CA-C-N	5.15	125.65	119.94
1	A	331	LEU	C-N-CA	5.15	125.65	119.94
2	C	26	GLY	CA-C-O	-5.10	116.95	122.05

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	3105	0	3201	10	0
1	B	3068	0	3164	14	0
2	C	901	0	861	7	0
2	D	910	0	872	5	0
3	A	25	0	0	0	0
3	B	25	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	128	0	178	1	0
5	B	78	0	111	0	0
6	A	8	0	0	0	0
6	B	11	0	0	0	0
6	C	6	0	0	0	0
6	D	4	0	0	0	0
All	All	8271	0	8387	36	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 (36) 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:B:320:VAL:HG13	1:B:324:LEU:HD23	1.73	0.71
1:A:320:VAL:HG13	1:A:324:LEU:HD23	1.75	0.67
1:B:227:TYR:HB3	1:B:292:LEU:HD11	1.83	0.60
1:B:238:ILE:HD11	1:B:285:GLU:HG2	1.85	0.57
5:A:507:2CV:H431	1:B:81:THR:HG21	1.85	0.56
1:B:177:ILE:HA	1:B:182:TRP:CD1	2.41	0.55
2:C:20:LEU:HG	2:C:82:MET:HE2	1.89	0.55
1:B:1072:ILE:HD12	1:B:1077:THR:HG21	1.92	0.52
2:D:28:ILE:HG22	2:D:32:ASN:HD22	1.75	0.52
1:B:1081:PHE:CE1	1:B:1086:VAL:HG22	2.44	0.52
2:C:28:ILE:HG22	2:C:32:ASN:HD22	1.76	0.51
2:D:20:LEU:HG	2:D:82:MET:HE2	1.92	0.51
1:A:1072:ILE:HD12	1:A:1077:THR:HG21	1.94	0.49
2:C:18:LEU:HB2	2:C:82:MET:HE3	1.95	0.49
1:B:1072:ILE:HG23	1:B:1077:THR:HG21	1.94	0.49
1:A:115:GLU:OE2	1:A:183:ARG:NH2	2.46	0.48
1:A:177:ILE:HA	1:A:182:TRP:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LEU:HD12	1:B:50:LEU:HD21	1.95	0.47
1:A:1072:ILE:HG23	1:A:1077:THR:HG21	1.97	0.46
2:C:11:LEU:HD23	2:C:117:THR:HB	1.98	0.46
1:B:1053:LEU:HD23	1:B:1107:LEU:HD11	1.99	0.45
2:D:11:LEU:HD23	2:D:117:THR:HB	1.99	0.45
2:C:90:THR:HG23	2:C:117:THR:HA	1.99	0.44
1:B:172:VAL:HG21	1:B:214:ILE:HG21	1.99	0.43
1:A:172:VAL:HG21	1:A:214:ILE:HG21	2.00	0.43
2:D:18:LEU:HB2	2:D:82:MET:HE3	2.01	0.43
1:A:175:LEU:HB3	1:A:176:PRO:HD3	2.01	0.42
2:D:90:THR:HG23	2:D:117:THR:HA	2.01	0.42
1:A:78:LEU:HD21	1:A:159:LYS:HE3	2.01	0.41
1:B:1016:VAL:HG12	1:B:1081:PHE:HD2	1.84	0.41
1:A:1028:TRP:HB2	1:A:1035:SER:HB2	2.03	0.41
1:A:205:ARG:HG3	1:A:314:VAL:HG13	2.03	0.41
2:C:32:ASN:OD1	2:C:71:ARG:NH2	2.47	0.41
1:B:140:TYR:CB	1:B:226:VAL:HG13	2.52	0.40
1:B:140:TYR:HB2	1:B:226:VAL:HG13	2.04	0.40
2:C:28:ILE:CG2	2:C:32:ASN:HD22	2.35	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	393/416 (94%)	384 (98%)	9 (2%)	0	100	100
1	B	385/416 (92%)	374 (97%)	11 (3%)	0	100	100
2	C	117/121 (97%)	113 (97%)	4 (3%)	0	100	100
2	D	118/121 (98%)	113 (96%)	5 (4%)	0	100	100
All	All	1013/1074 (94%)	984 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	333/354 (94%)	331 (99%)	2 (1%)	78	91
1	B	330/354 (93%)	328 (99%)	2 (1%)	78	91
2	C	94/96 (98%)	91 (97%)	3 (3%)	34	64
2	D	95/96 (99%)	92 (97%)	3 (3%)	34	64
All	All	852/900 (95%)	842 (99%)	10 (1%)	63	84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	VAL
1	A	292	LEU
2	C	17	SER
2	C	30	SER
2	C	56	SER
1	B	226	VAL
1	B	318	ASP
2	D	17	SER
2	D	30	SER
2	D	56	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1006	HIS
1	A	310	ASN
1	A	335	ASN
2	C	52	HIS
2	C	115	GLN
1	B	1059	ASN
2	D	5	GLN

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Mol	Chain	Res	Type
2	D	13	GLN
2	D	96	ASN
2	D	115	GLN

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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z > 2$
5	2CV	B	504	-	25,25,25	0.43	0	29,30,30	1.25	1 (3%)
5	2CV	A	503	-	25,25,25	0.34	0	29,30,30	0.86	1 (3%)
5	2CV	A	506	-	25,25,25	0.37	0	29,30,30	1.20	3 (10%)
5	2CV	A	507	-	25,25,25	0.44	0	29,30,30	1.01	2 (6%)
3	H98	A	501	-	26,26,26	0.39	0	31,34,34	0.62	0
5	2CV	B	505	-	25,25,25	0.39	0	29,30,30	1.13	2 (6%)
5	2CV	B	503	-	25,25,25	0.33	0	29,30,30	0.88	1 (3%)
3	H98	B	501	-	26,26,26	0.31	0	31,34,34	0.65	0
5	2CV	A	505	-	23,23,25	0.36	0	27,28,30	1.40	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	2CV	A	504	-	25,25,25	0.37	0	29,30,30	1.11	4 (13%)

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
5	2CV	B	504	-	-	11/34/34/34	-
5	2CV	A	503	-	-	8/34/34/34	-
5	2CV	A	506	-	-	7/34/34/34	-
5	2CV	A	507	-	-	10/34/34/34	-
3	H98	A	501	-	-	5/18/18/18	0/2/2/2
5	2CV	B	505	-	-	7/34/34/34	-
5	2CV	B	503	-	-	9/34/34/34	-
3	H98	B	501	-	-	4/18/18/18	0/2/2/2
5	2CV	A	505	-	-	13/32/32/34	-
5	2CV	A	504	-	-	10/34/34/34	-

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	504	2CV	C37-C40-C41	5.65	121.15	112.48
5	A	505	2CV	C37-C40-C41	5.36	120.72	112.48
5	B	505	2CV	C36-C37-C40	3.49	119.13	109.66
5	A	503	2CV	C36-C37-C40	3.33	118.69	109.66
5	A	507	2CV	C35-N33-C36	3.32	119.89	116.14
5	A	506	2CV	C37-C40-C41	2.99	117.06	112.48
5	B	505	2CV	C37-C40-C41	2.85	116.85	112.48
5	A	504	2CV	C36-C37-C40	2.82	117.30	109.66
5	A	504	2CV	C24-C27-C30	2.48	119.08	112.66
5	A	505	2CV	C36-C37-C40	2.48	116.37	109.66
5	B	503	2CV	C37-C40-C41	2.41	116.18	112.48
5	A	507	2CV	C37-C40-C41	2.39	116.15	112.48
5	A	504	2CV	C37-C40-C41	2.36	116.11	112.48
5	A	506	2CV	C36-C37-C40	2.18	115.56	109.66
5	A	506	2CV	C27-C30-N33	2.18	121.39	118.09
5	A	504	2CV	C35-N33-C36	2.17	118.60	116.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	505	2CV	C43-C42-C41	2.10	116.44	112.17

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	H98	C1-C2-C3-C4
3	A	501	H98	N1-C2-C3-C4
3	A	501	H98	O3-C19-N2-C15
3	B	501	H98	N1-C2-C3-C4
3	B	501	H98	O3-C19-N2-C15
5	A	503	2CV	C36-C37-C40-C41
5	A	503	2CV	C36-C37-C40-O49
5	A	504	2CV	C37-C36-N33-C35
5	A	505	2CV	N33-C36-C37-O47
5	A	505	2CV	C40-C41-C42-C43
5	A	505	2CV	O51-C41-C42-C43
5	A	505	2CV	O51-C41-C42-O53
5	A	507	2CV	C60-C35-N33-C36
5	B	504	2CV	N33-C36-C37-C40
5	B	504	2CV	N33-C36-C37-O47
5	B	505	2CV	C41-C42-C43-O44
5	B	505	2CV	O53-C42-C43-O44
5	A	504	2CV	O34-C30-N33-C36
5	A	504	2CV	O53-C42-C43-O44
3	A	501	H98	C8-C7-O1-C10
3	A	501	H98	C6-C7-O1-C10
3	B	501	H98	C6-C7-O1-C10
3	B	501	H98	C8-C7-O1-C10
5	A	505	2CV	O34-C30-N33-C36
5	A	507	2CV	C60-C35-N33-C30
5	A	506	2CV	C60-C35-N33-C36
5	A	507	2CV	O34-C30-N33-C36
5	A	504	2CV	O34-C30-N33-C35
5	B	504	2CV	O34-C30-N33-C36
5	B	503	2CV	C24-C27-C30-O34
5	A	504	2CV	C41-C42-C43-O44
5	A	504	2CV	C27-C30-N33-C36
5	A	505	2CV	C27-C30-N33-C36
5	A	505	2CV	C24-C27-C30-N33
5	A	505	2CV	C24-C27-C30-O34
5	A	504	2CV	C37-C36-N33-C30

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Mol	Chain	Res	Type	Atoms
5	B	505	2CV	O51-C41-C42-O53
5	A	505	2CV	C40-C41-C42-O53
5	B	505	2CV	C40-C41-C42-O53
5	A	506	2CV	C60-C35-N33-C30
5	B	503	2CV	C24-C27-C30-N33
5	A	505	2CV	O34-C30-N33-C35
5	A	503	2CV	O47-C37-C40-O49
5	A	506	2CV	C15-C18-C21-C24
5	B	503	2CV	C60-C35-N33-C36
5	A	503	2CV	C27-C30-N33-C36
5	A	507	2CV	C27-C30-N33-C36
5	B	504	2CV	C27-C30-N33-C36
5	A	506	2CV	C12-C15-C18-C21
5	A	503	2CV	N33-C35-C60-O63
5	B	505	2CV	C40-C41-C42-C43
5	A	507	2CV	O34-C30-N33-C35
5	A	505	2CV	N33-C35-C60-O63
5	A	503	2CV	C12-C15-C18-C21
5	B	504	2CV	O53-C42-C43-O44
5	B	504	2CV	C15-C18-C21-C24
5	B	503	2CV	N33-C35-C60-O63
5	B	505	2CV	O51-C41-C42-C43
5	A	503	2CV	O47-C37-C40-C41
5	A	507	2CV	C15-C18-C21-C24
5	A	506	2CV	C15-C12-C9-C1
5	A	503	2CV	C15-C12-C9-C1
5	B	503	2CV	C18-C21-C24-C27
5	A	504	2CV	C27-C30-N33-C35
5	A	505	2CV	N33-C36-C37-C40
5	B	503	2CV	C15-C18-C21-C24
5	B	504	2CV	C40-C41-C42-O53
5	B	504	2CV	O34-C30-N33-C35
5	B	503	2CV	C15-C12-C9-C1
5	A	504	2CV	C0-C1-C9-C12
5	A	505	2CV	C27-C30-N33-C35
5	B	503	2CV	C12-C15-C18-C21
5	A	506	2CV	C9-C12-C15-C18
5	B	505	2CV	N33-C35-C60-O63
5	A	507	2CV	C27-C30-N33-C35
5	B	504	2CV	C27-C30-N33-C35
5	B	503	2CV	C60-C35-N33-C30
5	A	507	2CV	C15-C12-C9-C1

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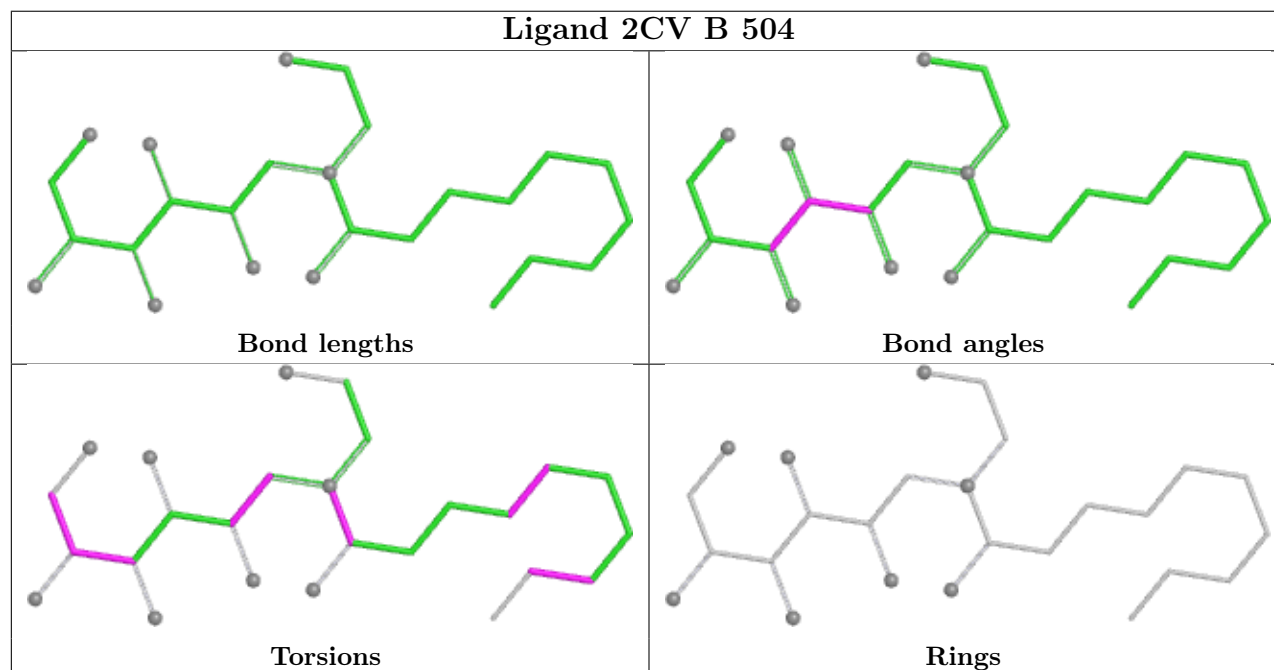
Mol	Chain	Res	Type	Atoms
5	A	506	2CV	C21-C24-C27-C30
5	B	504	2CV	C0-C1-C9-C12
5	B	504	2CV	O51-C41-C42-O53
5	A	507	2CV	C12-C15-C18-C21
5	A	507	2CV	C9-C12-C15-C18
5	A	504	2CV	N33-C35-C60-O63

There are no ring outliers.

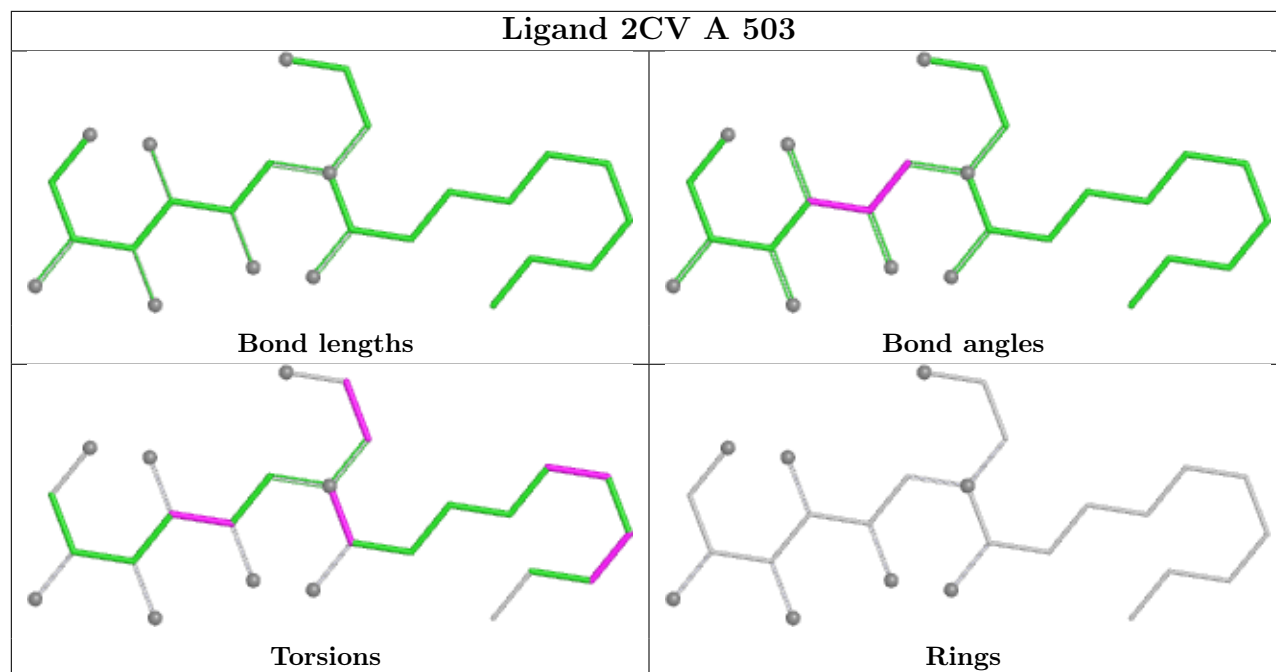
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	507	2CV	1	0

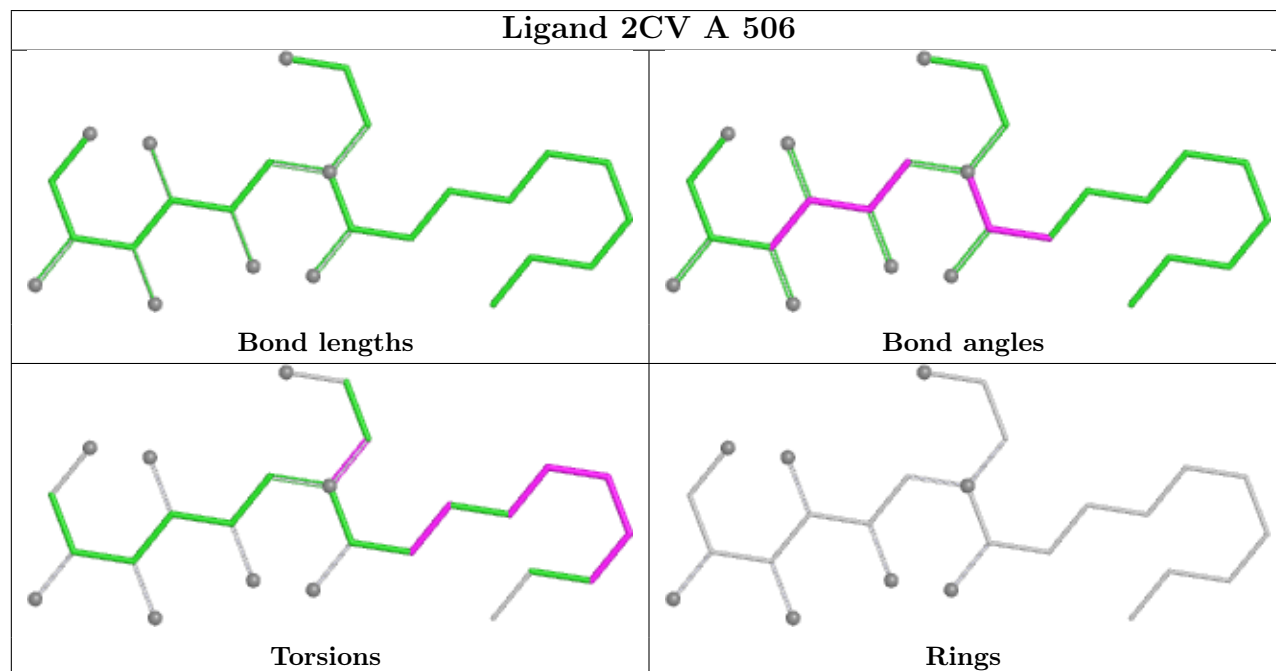
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



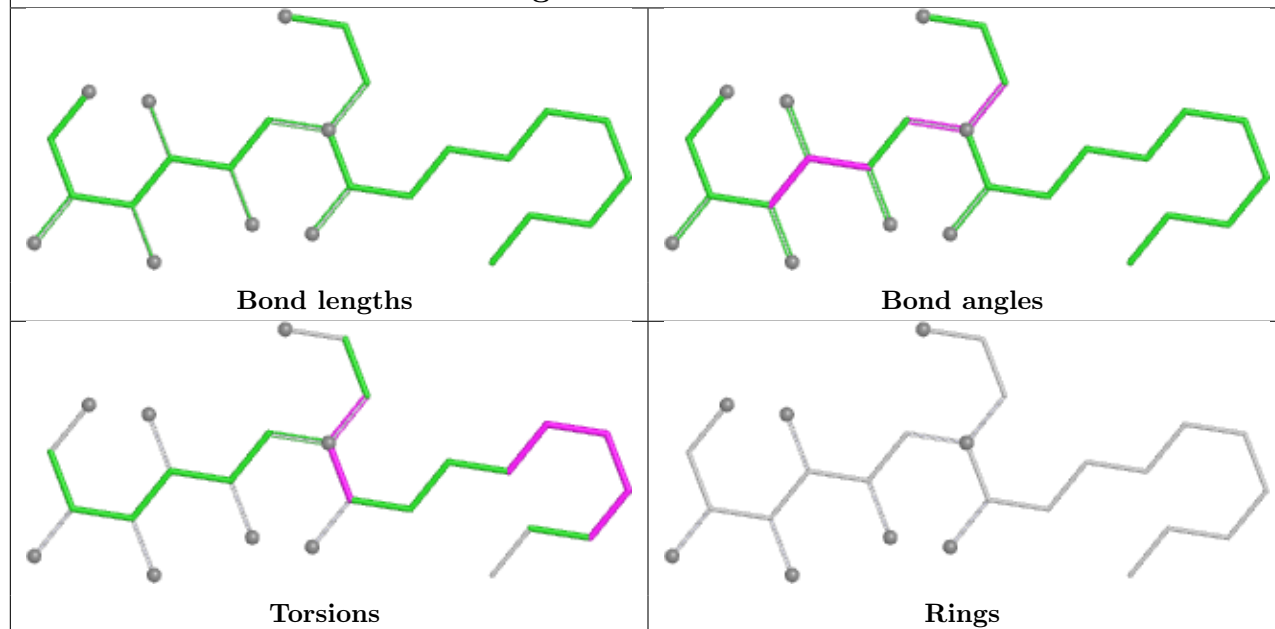
Ligand 2CV A 503



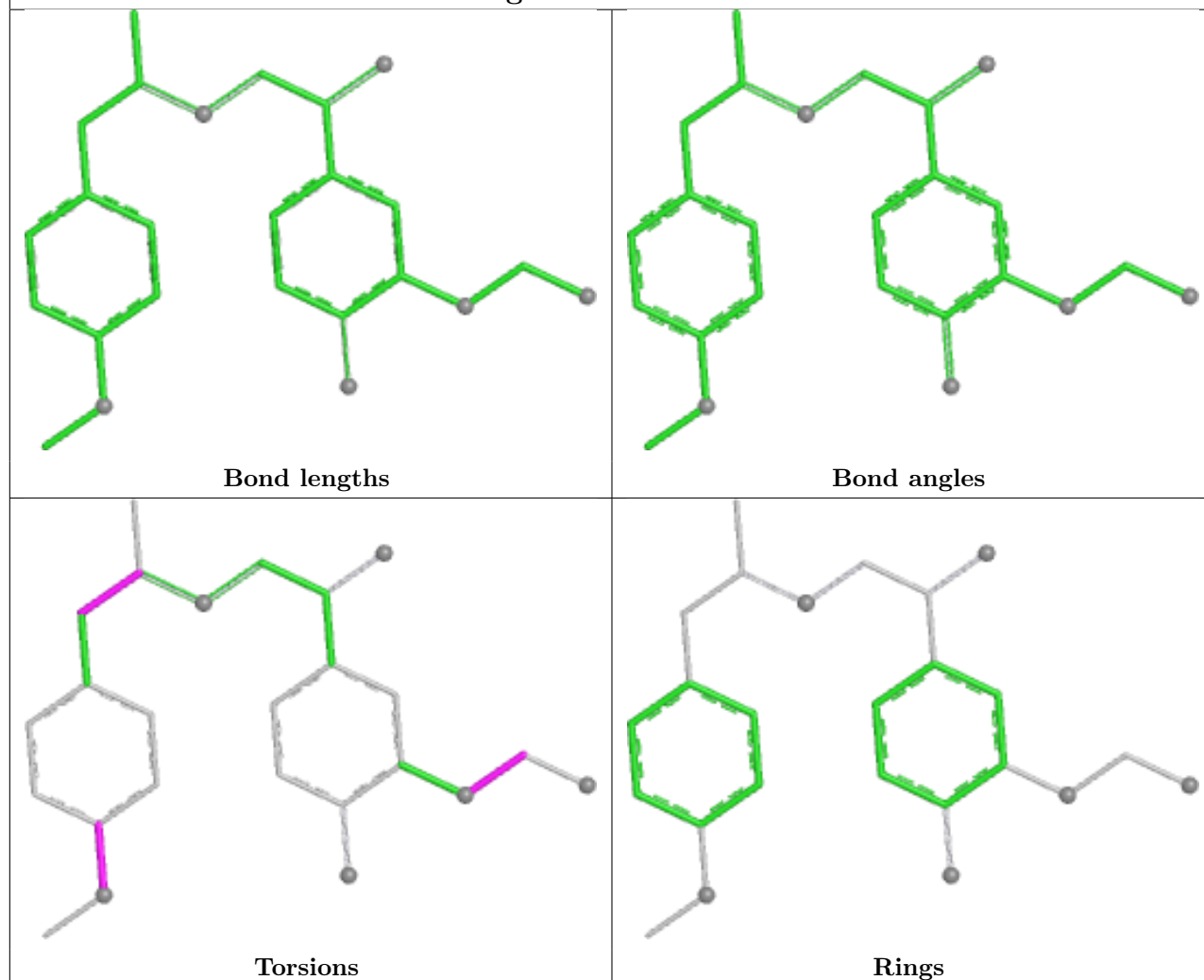
Ligand 2CV A 506

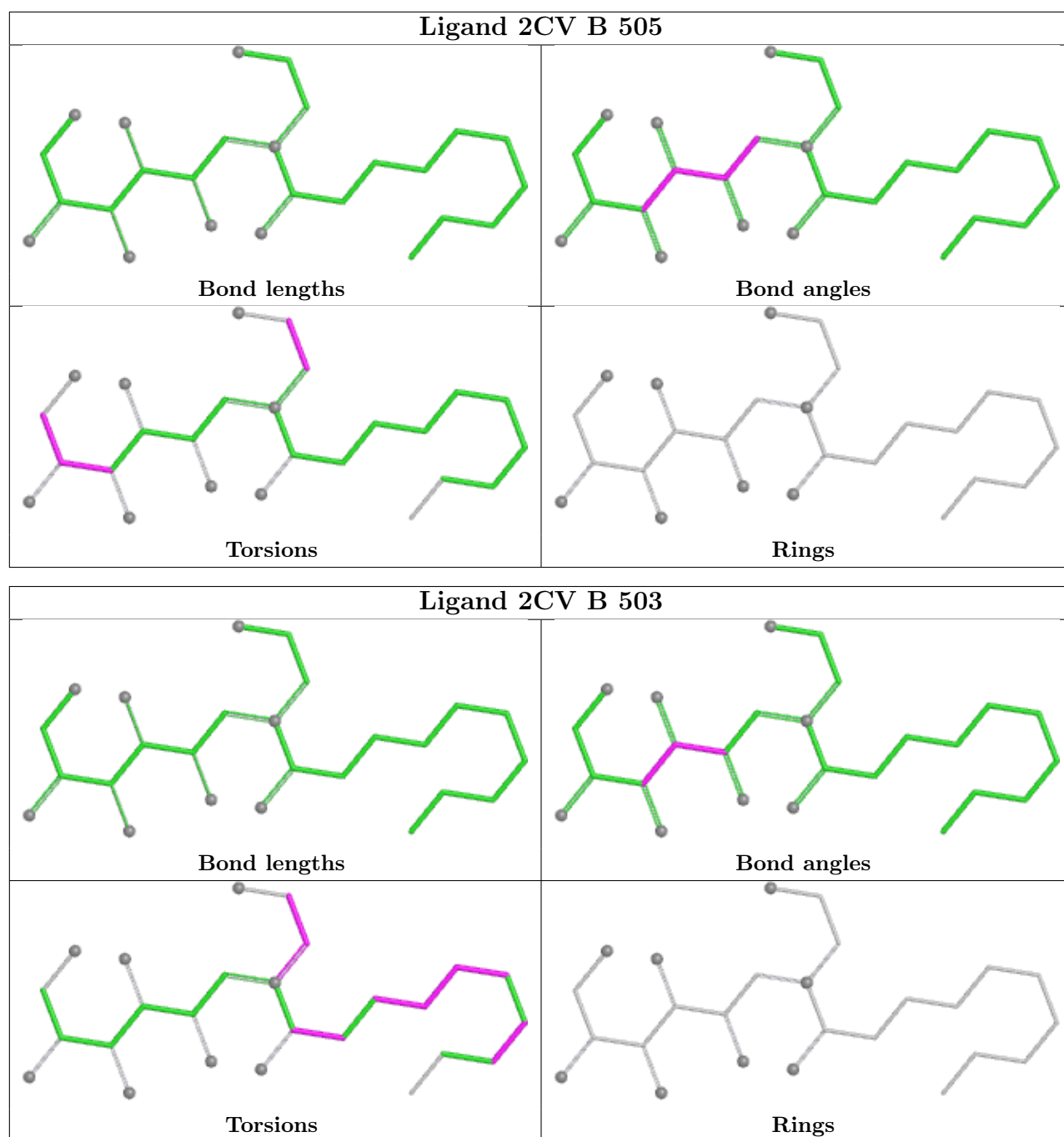


Ligand 2CV A 507

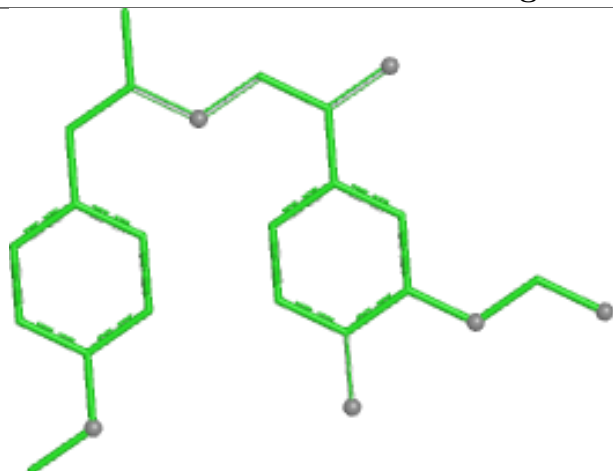


Ligand H98 A 501

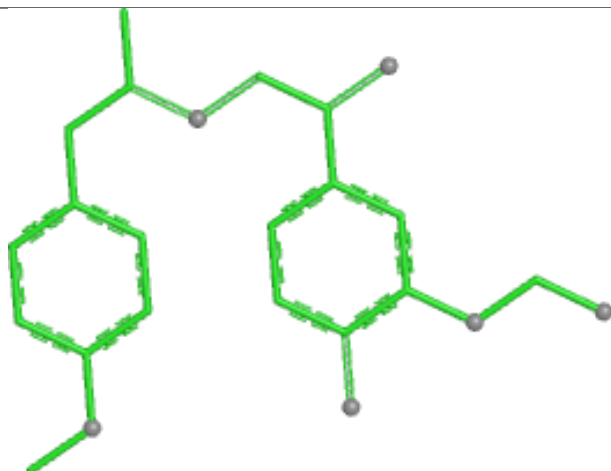




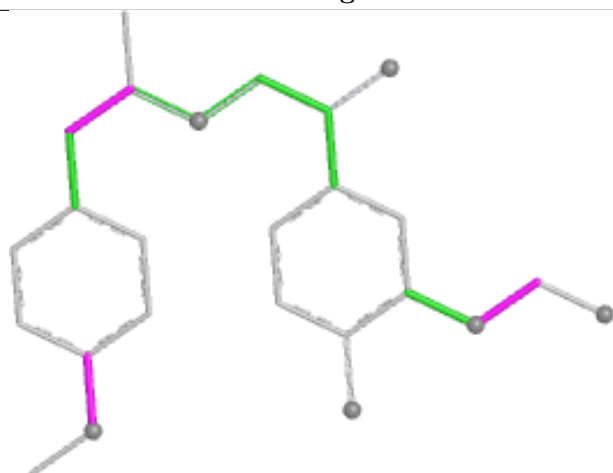
Ligand H98 B 501



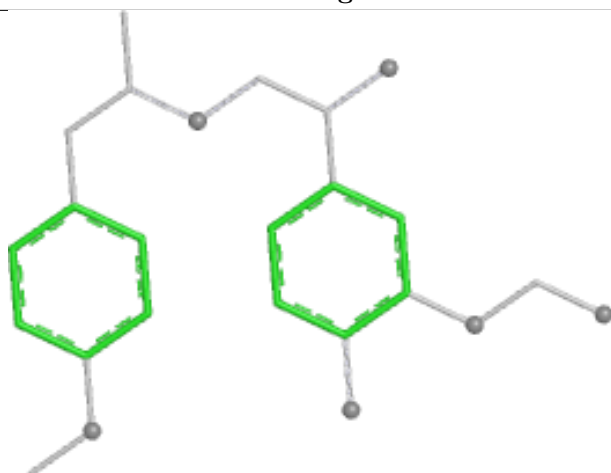
Bond lengths



Bond angles

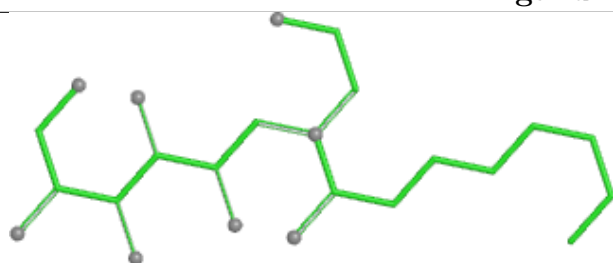


Torsions

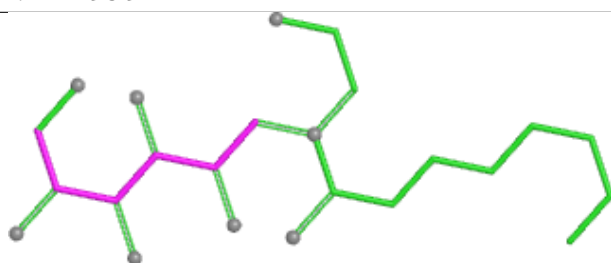


Rings

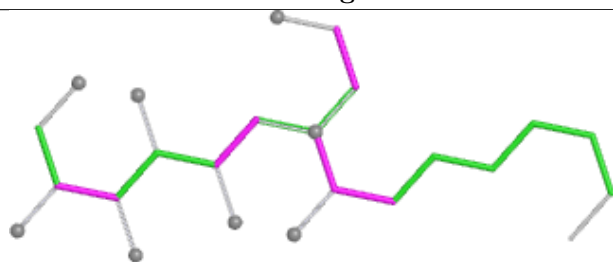
Ligand 2CV A 505



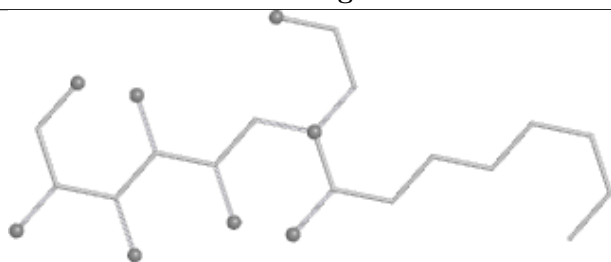
Bond lengths



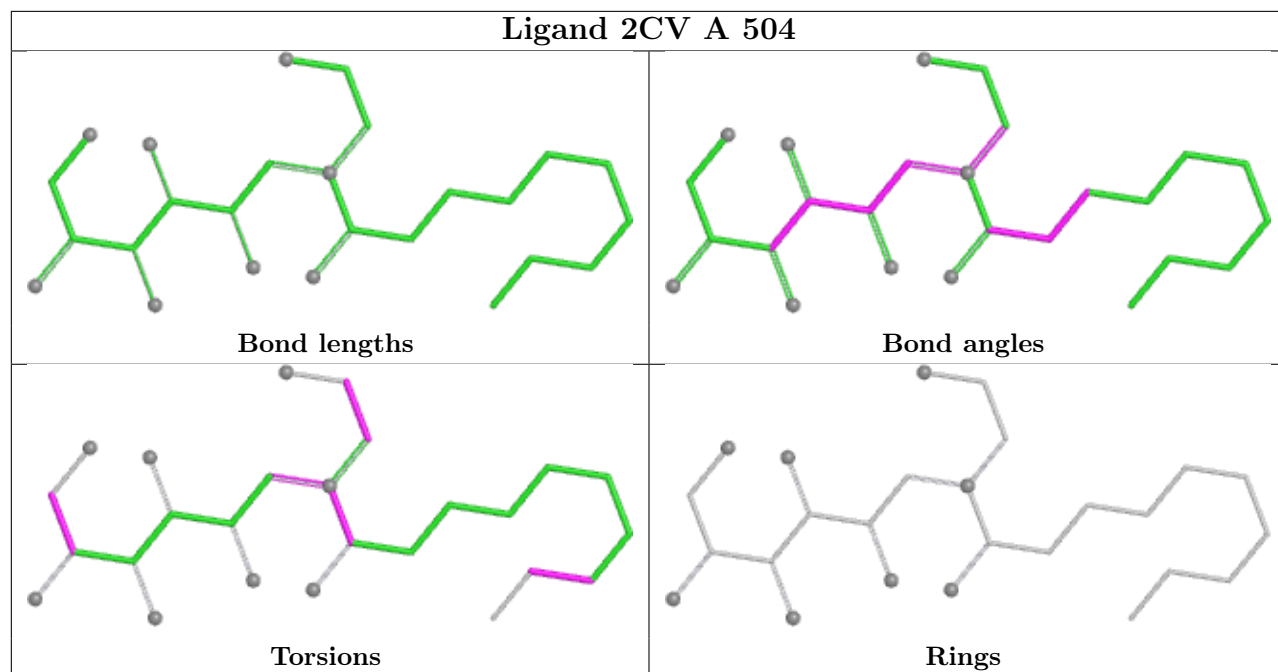
Bond angles



Torsions



Rings



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	397/416 (95%)	1.02	80 (20%) 3 2	30, 72, 138, 182	0
1	B	391/416 (93%)	1.41	97 (24%) 2 1	35, 73, 117, 142	0
2	C	119/121 (98%)	0.48	11 (9%) 14 12	30, 48, 82, 100	0
2	D	120/121 (99%)	0.63	15 (12%) 8 7	36, 60, 95, 112	0
All	All	1027/1074 (95%)	1.06	203 (19%) 3 2	30, 66, 122, 182	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	ARG	7.7
1	A	1088	ALA	7.3
1	B	188	GLN	6.8
1	A	194	GLN	6.7
1	B	1055	VAL	6.2
2	D	13	GLN	6.0
1	B	272	ALA	5.9
1	B	1002	ASP	5.7
1	A	1040	PRO	5.7
1	A	1078	LEU	5.4
1	A	111	SER	5.3
1	A	1080	LEU	5.2
1	B	239	ARG	5.2
1	B	1080	LEU	5.2
1	A	1109	GLU	5.2
1	B	1106	ASN	5.1
1	B	1108	ALA	5.1
1	B	1060	ILE	4.9
1	B	1051	GLY	4.8
2	C	88	GLU	4.8
1	A	1087	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	1015	ASP	4.7
1	B	1014	THR	4.7
1	B	315	PHE	4.7
1	B	1087	ALA	4.6
1	A	1079	LEU	4.6
2	D	1	GLN	4.6
1	B	1073	ARG	4.5
2	C	41	PRO	4.4
1	B	1016	VAL	4.4
1	A	108	LEU	4.4
1	B	1022	ALA	4.3
1	B	1040	PRO	4.3
2	C	25	SER	4.2
1	B	273	SER	4.2
1	B	282	ALA	4.1
1	B	242	ASP	4.1
1	B	1105	ALA	4.0
1	A	1090	LYS	4.0
1	B	1052	LYS	4.0
1	B	1042	LEU	4.0
1	A	315	PHE	4.0
1	A	358	ALA	4.0
1	A	1089	THR	3.9
1	B	1089	THR	3.9
1	B	116	LEU	3.9
1	B	345	ARG	3.9
1	B	1020	ASP	3.8
1	B	317	ARG	3.8
2	D	42	GLY	3.8
2	D	41	PRO	3.8
1	B	322	ASP	3.8
2	C	11	LEU	3.7
2	D	14	ALA	3.7
2	D	43	LYS	3.7
1	B	1023	ILE	3.7
1	A	1070	TYR	3.7
1	B	1036	LYS	3.7
1	A	1091	VAL	3.7
1	B	1019	ALA	3.6
1	B	120	LEU	3.6
1	A	1026	ASP	3.6
1	A	1013	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1108	ALA	3.5
1	B	109	TRP	3.5
1	B	90	VAL	3.5
1	A	1031	TRP	3.5
1	B	241	ILE	3.5
1	B	240	LYS	3.4
1	A	1039	ALA	3.4
1	A	205	ARG	3.3
1	A	1086	VAL	3.3
1	A	195	ASP	3.3
1	A	189	ALA	3.3
1	B	313	ASN	3.3
1	A	148	ARG	3.2
1	A	1077	THR	3.2
1	B	1082	LYS	3.2
2	D	114	THR	3.2
2	C	75	ALA	3.2
1	B	1091	VAL	3.2
1	A	104	ARG	3.1
1	A	109	TRP	3.1
1	B	149	TYR	3.1
1	A	1067	ALA	3.1
1	B	1088	ALA	3.1
1	A	1051	GLY	3.0
1	B	88	LEU	3.0
1	A	1050	GLN	3.0
2	D	120	SER	3.0
1	B	1054	THR	3.0
1	B	238	ILE	3.0
1	A	334	ALA	3.0
1	B	1053	LEU	3.0
1	B	1056	ALA	2.9
1	B	123	LEU	2.9
1	B	319	LEU	2.9
2	C	87	PRO	2.9
1	A	1037	MET	2.9
1	A	243	ARG	2.9
1	B	1043	ASP	2.9
2	C	73	ASN	2.8
1	A	193	TYR	2.8
1	A	112	PHE	2.8
1	B	185	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	188	GLN	2.8
1	B	316	ASN	2.8
1	A	50	LEU	2.8
1	A	318	ASP	2.8
1	B	1109	GLU	2.8
1	B	358	ALA	2.8
1	A	190	LEU	2.7
1	B	91	GLY	2.7
1	A	1014	THR	2.7
1	A	1047	ASP	2.7
1	B	205	ARG	2.7
1	B	103	VAL	2.7
1	A	345	ARG	2.7
1	B	1083	ASN	2.7
1	B	41	ALA	2.7
1	B	1033	GLY	2.6
1	B	1003	LYS	2.6
1	A	1012	PHE	2.6
1	A	187	PRO	2.6
1	A	1043	ASP	2.6
1	A	47	LEU	2.6
1	B	1024	LEU	2.6
1	B	190	LEU	2.6
1	B	286	HIS	2.6
1	A	1066	THR	2.5
1	B	119	SER	2.5
2	C	72	ASP	2.5
1	B	55	ILE	2.5
1	A	191	LYS	2.5
1	B	1100	LYS	2.5
1	A	41	ALA	2.5
1	B	1062	GLN	2.5
1	B	84	ALA	2.5
1	B	318	ASP	2.5
1	B	341	ILE	2.5
1	A	1085	GLU	2.5
1	B	1046	ALA	2.5
1	B	157	ARG	2.5
1	A	1025	VAL	2.5
1	A	1081	PHE	2.5
1	B	234	ALA	2.5
1	A	1069	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	89	VAL	2.4
2	D	30	SER	2.4
1	A	1034	PRO	2.4
1	B	170	ALA	2.4
1	B	1047	ASP	2.4
1	A	196	PRO	2.4
1	A	1021	GLY	2.4
1	B	1079	LEU	2.3
1	B	193	TYR	2.3
1	B	283	MET	2.3
1	A	1094	LEU	2.3
1	A	46	LEU	2.3
1	B	356	LEU	2.3
1	A	283	MET	2.3
1	A	287	LYS	2.3
1	A	1084	GLY	2.3
1	B	1070	TYR	2.3
1	A	1011	SER	2.3
1	B	183	ARG	2.3
2	D	75	ALA	2.3
1	B	1085	GLU	2.3
2	C	76	ASN	2.3
1	A	1068	PRO	2.3
1	A	317	ARG	2.3
1	B	348	ASP	2.3
1	B	323	TRP	2.3
1	A	280	VAL	2.3
2	D	40	ALA	2.2
1	A	176	PRO	2.2
2	D	27	SER	2.2
1	B	43	VAL	2.2
1	B	60	VAL	2.2
1	A	44	MET	2.2
1	B	75	LEU	2.2
1	B	184	ASP	2.2
2	D	2	VAL	2.2
1	B	115	GLU	2.1
1	A	1023	ILE	2.1
2	C	24	ALA	2.1
1	A	182	TRP	2.1
1	A	1103	LEU	2.1
1	A	110	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	149	TYR	2.1
1	A	314	VAL	2.1
2	D	74	ALA	2.1
1	A	354	LYS	2.1
1	B	1103	LEU	2.1
1	B	308	LEU	2.1
1	A	105	GLY	2.1
1	B	1044	GLU	2.0
2	C	40	ALA	2.0
1	A	284	LYS	2.0
1	A	150	GLN	2.0
1	B	177	ILE	2.0
1	A	1027	PHE	2.0
2	D	104	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	2CV	A	506	26/26	0.72	0.22	45,59,81,86	0
5	2CV	B	504	26/26	0.75	0.29	55,74,89,118	0
5	2CV	B	505	26/26	0.80	0.24	72,89,107,131	0
5	2CV	A	507	26/26	0.82	0.20	50,63,66,71	0
5	2CV	B	503	26/26	0.85	0.16	72,80,103,120	0
5	2CV	A	504	26/26	0.86	0.24	52,104,124,132	0
4	NA	A	502	1/1	0.87	0.09	79,79,79,79	0
5	2CV	A	503	26/26	0.90	0.15	48,68,78,80	0
5	2CV	A	505	24/26	0.91	0.14	64,91,97,99	0

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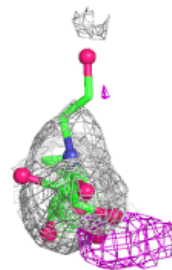
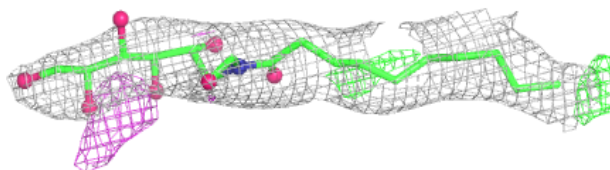
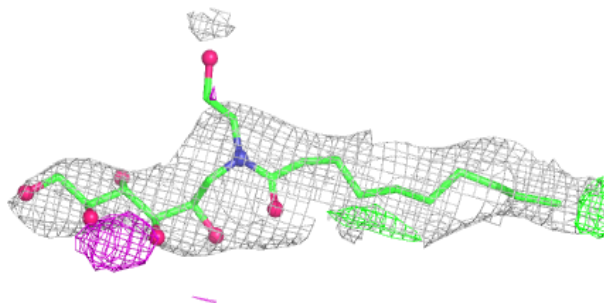
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	H98	B	501	25/25	0.93	0.12	54,60,70,76	0
3	H98	A	501	25/25	0.94	0.10	45,54,64,65	0
4	NA	B	502	1/1	0.96	0.05	68,68,68,68	0

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.

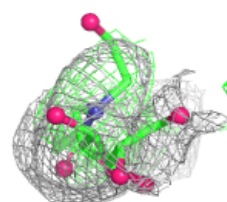
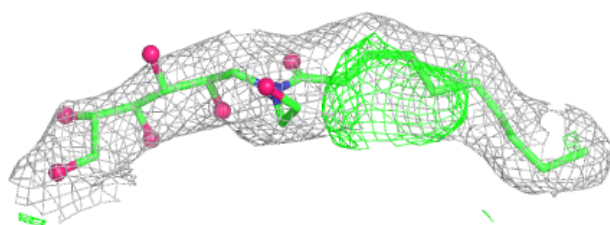
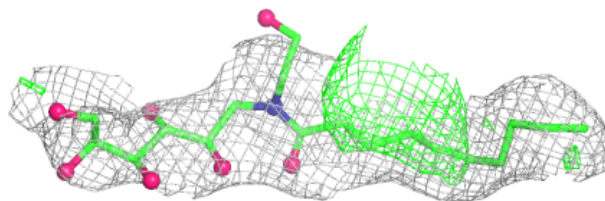
Electron density around 2CV A 506:

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

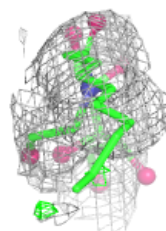
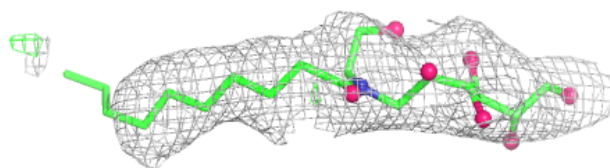
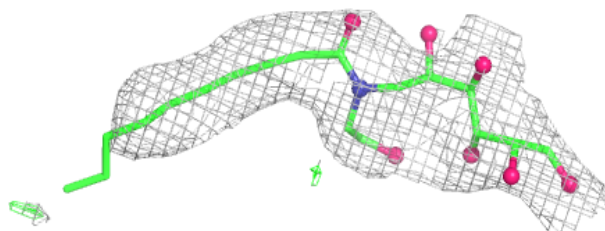


Electron density around 2CV B 504:

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

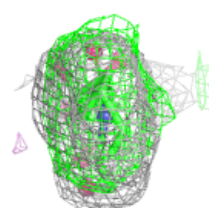
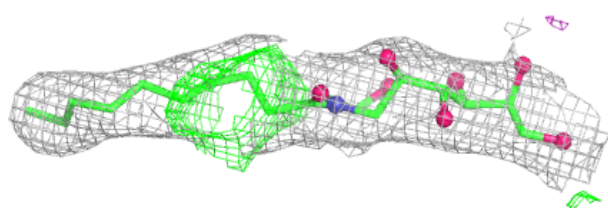
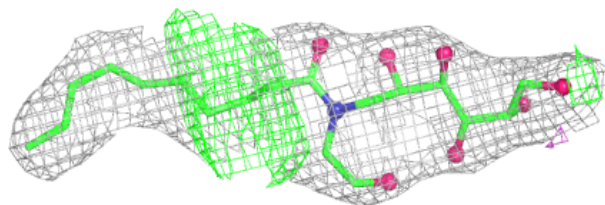
**Electron density around 2CV B 505:**

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

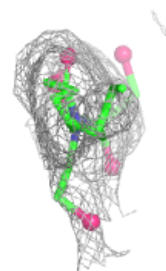
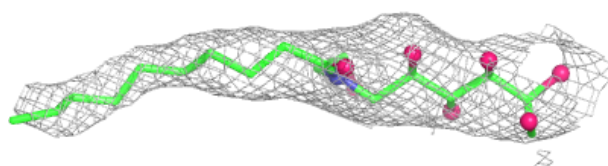


Electron density around 2CV A 507:

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

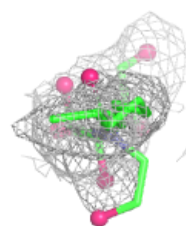
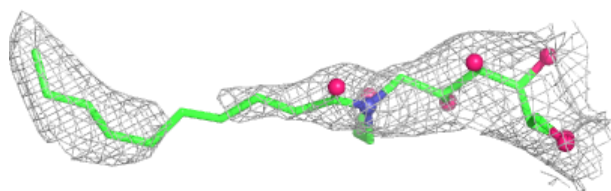
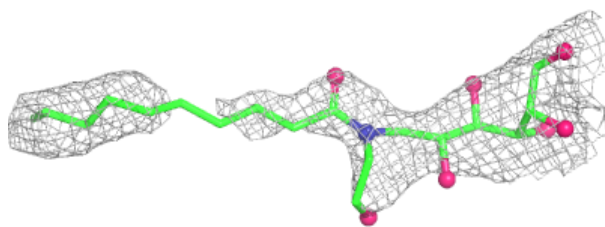
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

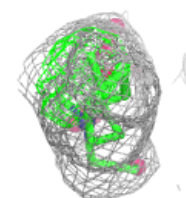
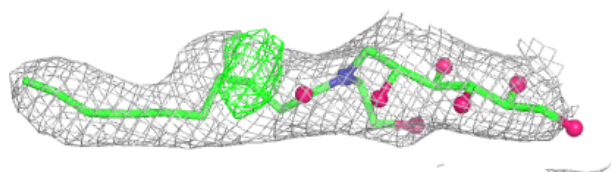
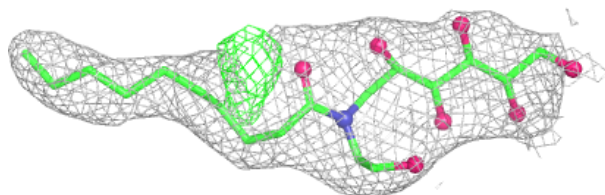


Electron density around 2CV A 504:

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

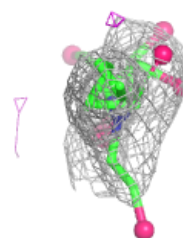
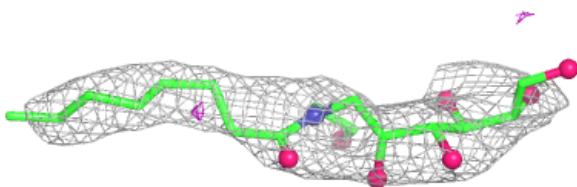
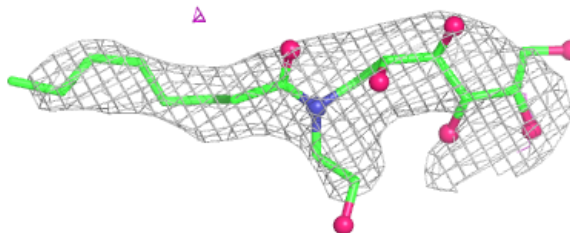
**Electron density around 2CV A 503:**

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

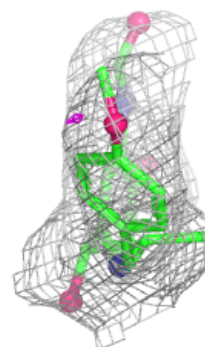
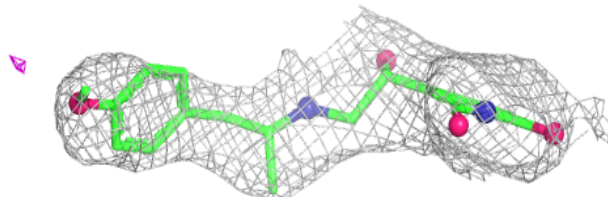
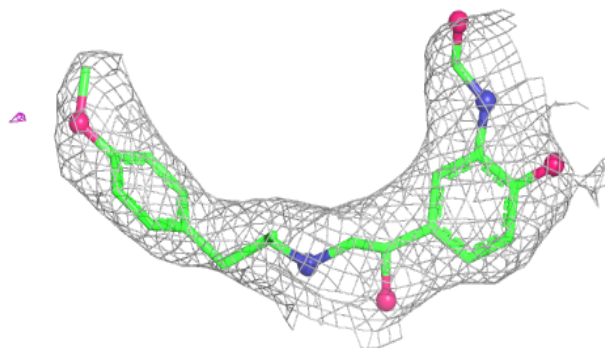


Electron density around 2CV A 505:

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

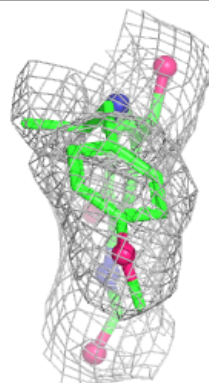
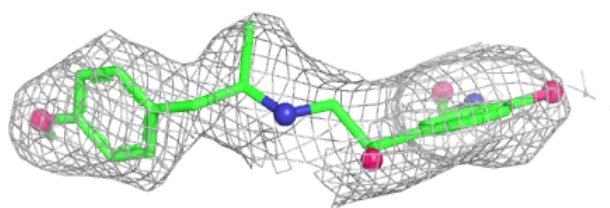
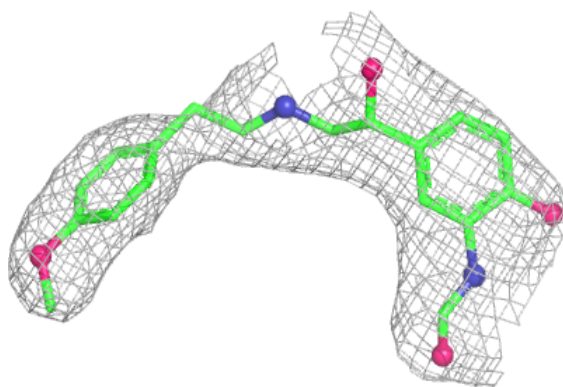
**Electron density around H98 B 501:**

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



Electron density around H98 A 501:

$2mF_o-DF_c$ (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.