



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:46 PM UTC

PDB ID : 6B73 / pdb_00006b73
Title : Crystal Structure of a nanobody-stabilized active state of the kappa-opioid receptor
Authors : Che, T.; Majumdar, S.; Zaidi, S.A.; Kormos, C.; McCorvy, J.D.; Wang, S.; Mosier, P.D.; Uprety, R.; Vardy, E.; Krumm, B.E.; Han, G.W.; Lee, M.Y.; Pardon, E.; Steyaert, J.; Huang, X.P.; Strachan, R.T.; Tribo, A.R.; Pasternak, G.W.; Carroll, I.F.; Stevens, R.C.; Cherezov, V.; Katritch, V.; Wacker, D.; Roth, B.L.
Deposited on : 2017-10-03
Resolution : 3.10 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

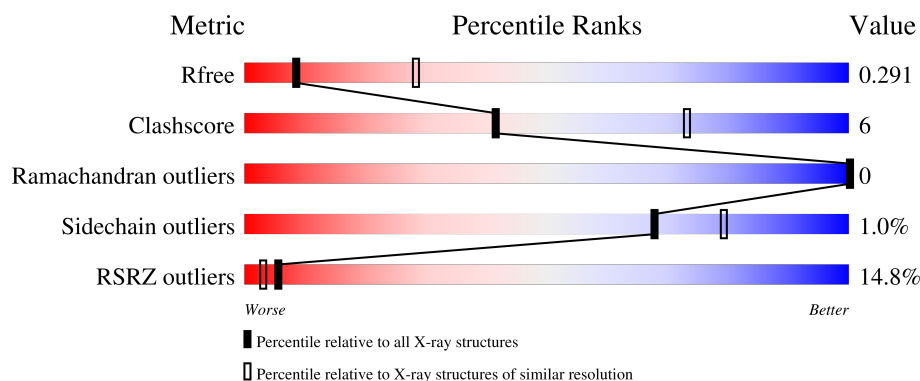
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	418	8% 58% 9% 33%
1	B	418	9% 56% 8% 36%
2	C	134	16% 83% 10% 6%

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	D	134	19% 79% 10% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6142 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 Soluble cytochrome b562, kappa-type opioid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2117	1415	322	364	16			
1	B	269	Total	C	N	O	S	0	0	0
			2013	1353	302	341	17			

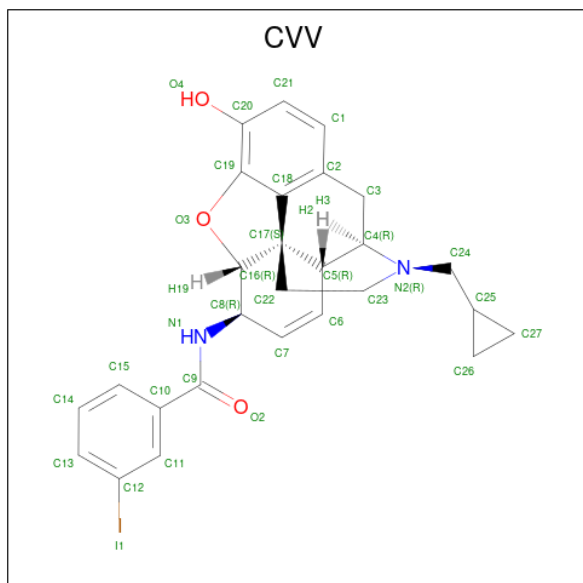
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-59	GLY	-	expression tag	UNP P0ABE7
A	-58	GLY	-	expression tag	UNP P0ABE7
A	-57	THR	-	expression tag	UNP P0ABE7
A	-56	THR	-	expression tag	UNP P0ABE7
A	-55	MET	-	expression tag	UNP P0ABE7
A	-48	TRP	MET	engineered mutation	UNP P0ABE7
A	47	ILE	HIS	engineered mutation	UNP P0ABE7
A	51	LEU	ARG	engineered mutation	UNP P0ABE7
A	52	GLY	-	linker	UNP P0ABE7
A	53	SER	-	linker	UNP P0ABE7
A	135	LEU	ILE	engineered mutation	UNP P41145
B	-59	GLY	-	expression tag	UNP P0ABE7
B	-58	GLY	-	expression tag	UNP P0ABE7
B	-57	THR	-	expression tag	UNP P0ABE7
B	-56	THR	-	expression tag	UNP P0ABE7
B	-55	MET	-	expression tag	UNP P0ABE7
B	-48	TRP	MET	engineered mutation	UNP P0ABE7
B	47	ILE	HIS	engineered mutation	UNP P0ABE7
B	51	LEU	ARG	engineered mutation	UNP P0ABE7
B	52	GLY	-	linker	UNP P0ABE7
B	53	SER	-	linker	UNP P0ABE7
B	135	LEU	ILE	engineered mutation	UNP P41145

- Molecule 2 is a protein called Nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	126	Total	C	N	O	S	0	0	0
			959	594	170	191	4			
2	D	122	Total	C	N	O	S	0	0	0
			917	570	163	180	4			

- Molecule 3 is N-[(5 α ,6 β)-17-(cyclopropylmethyl)-3-hydroxy-7,8-didehydro-4,5-epoxymorphinan-6-yl]-3-iodobenzamide (CCD ID: CVV) (formula: C₂₇H₂₇IN₂O₃) (labeled as "Ligand of Interest" by depositor).



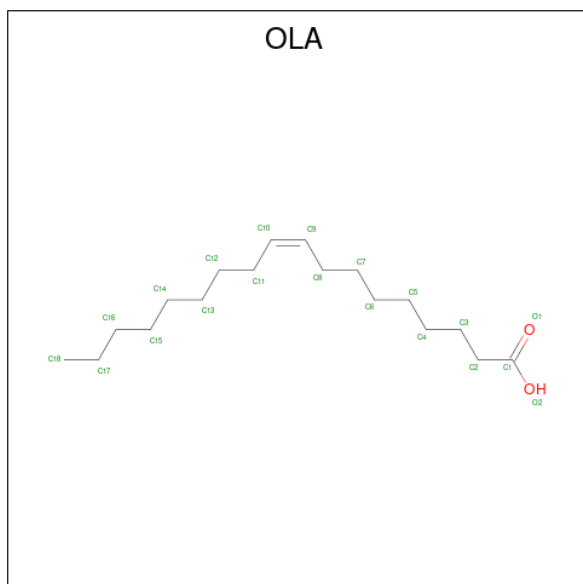
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	I	N	O	0	0
			33	27	1	2	3		
3	B	1	Total	C	I	N	O	0	0
			33	27	1	2	3		

- Molecule 4 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			28	27	1		
4	B	1	Total	C	O	0	0
			28	27	1		

- Molecule 5 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$) (labeled as "Ligand of Interest" by depositor).

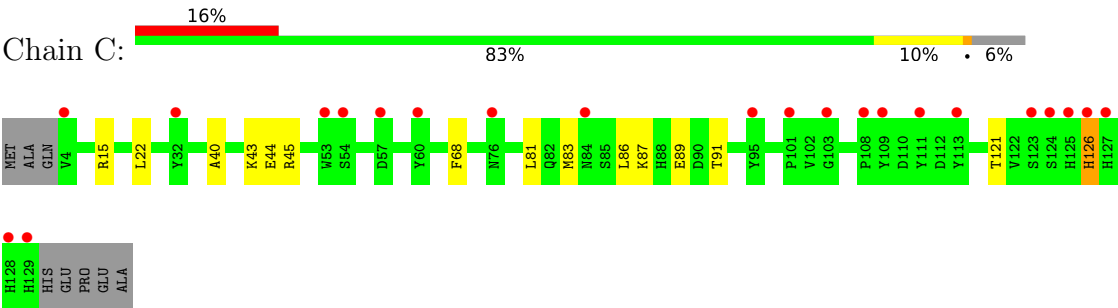


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			14	12	2		

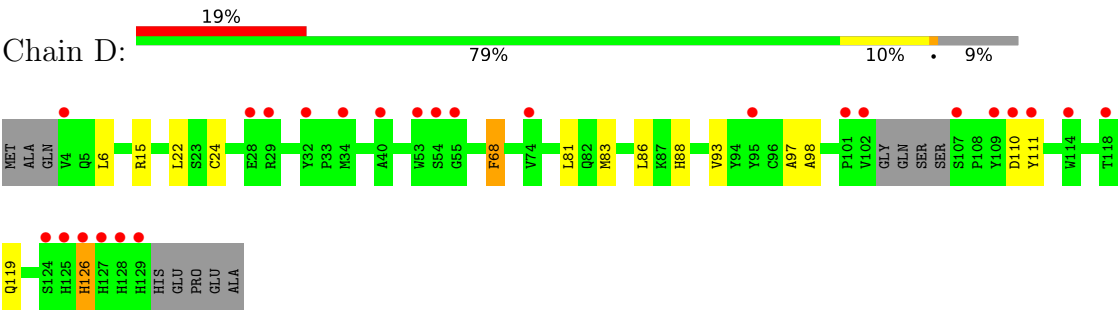
- Molecule 1: Soluble cytochrome b562, kappa-type opioid receptor



● Molecule 2: Nanobody



● Molecule 2: Nanobody



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.31Å 150.75Å 100.28Å 90.00° 105.66° 90.00°	Depositor
Resolution (Å)	46.94 – 3.10 46.94 – 3.10	Depositor EDS
% Data completeness (in resolution range)	93.5 (46.94-3.10) 93.5 (46.94-3.10)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.254 , 0.275 0.271 , 0.291	Depositor DCC
R_{free} test set	1505 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	76.3	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.057 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6142	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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: OLA, CVV, CLR

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	0.93	1/2167 (0.0%)	1.28	7/2970 (0.2%)
1	B	0.94	1/2060 (0.0%)	1.30	6/2830 (0.2%)
2	C	0.79	0/983	1.05	0/1339
2	D	0.76	0/940	1.04	0/1283
All	All	0.89	2/6150 (0.0%)	1.22	13/8422 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	ILE	CA-C	5.45	1.58	1.52
1	B	58	ILE	CA-CB	5.12	1.57	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	VAL	N-CA-C	7.71	118.25	110.23
1	A	306	THR	N-CA-C	-7.67	103.53	113.12
1	A	57	ALA	CA-C-N	6.26	124.18	120.24
1	A	57	ALA	C-N-CA	6.26	124.18	120.24
1	B	236	VAL	CB-CA-C	-6.12	103.87	111.70
1	B	57	ALA	CA-C-N	5.61	123.77	120.24
1	B	57	ALA	C-N-CA	5.61	123.77	120.24
1	A	116	SER	CA-C-N	5.38	127.43	120.44
1	A	116	SER	C-N-CA	5.38	127.43	120.44
1	B	148	THR	CA-C-N	5.32	127.41	120.28
1	B	148	THR	C-N-CA	5.32	127.41	120.28
1	A	148	THR	CA-C-N	5.25	127.32	120.28
1	A	148	THR	C-N-CA	5.25	127.32	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2117	0	2090	27	0
1	B	2013	0	1987	21	0
2	C	959	0	876	16	0
2	D	917	0	819	13	0
3	A	33	0	0	2	0
3	B	33	0	0	3	0
4	A	28	0	46	3	0
4	B	28	0	46	1	0
5	A	14	0	18	0	0
All	All	6142	0	5882	77	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 6.

All (77) 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:D:15:ARG:HG2	2:D:126:HIS:HB3	1.29	1.09
2:C:15:ARG:HG2	2:C:126:HIS:HB3	1.37	1.04
2:D:15:ARG:CG	2:D:126:HIS:HB3	2.16	0.74
2:C:15:ARG:CG	2:C:126:HIS:HB3	2.19	0.72
1:A:69:VAL:HB	1:A:112:MET:HE1	1.72	0.72
1:B:69:VAL:HB	1:B:112:MET:HE1	1.76	0.68
1:A:97:TYR:HB3	1:A:152:MET:HE2	1.75	0.68
2:D:6:LEU:HD21	2:D:98:ALA:HB2	1.75	0.68
1:A:237:ILE:HG13	1:A:238:PRO:HD3	1.74	0.67
1:A:285:VAL:HA	4:A:2002:CLR:H261	1.77	0.67
1:B:223:ASP:OD1	1:B:227:LYS:NZ	2.31	0.64
1:A:90:MET:O	1:A:90:MET:HG3	2.00	0.61
2:D:83:MET:HB3	2:D:86:LEU:HD21	1.84	0.59
2:C:83:MET:HB3	2:C:86:LEU:HD21	1.84	0.59
1:A:134:VAL:HG12	3:A:2001:CVV:I1	2.73	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:PHE:C	1:A:238:PRO:HD2	2.28	0.58
2:C:91:THR:HG23	2:C:121:THR:HA	1.86	0.58
1:B:90:MET:O	1:B:90:MET:HG3	2.02	0.58
1:B:134:VAL:HG12	3:B:2001:CVV:I1	2.73	0.57
1:A:208:ILE:HD12	1:A:208:ILE:H	1.71	0.56
2:D:15:ARG:NE	2:D:126:HIS:ND1	2.45	0.55
2:D:68:PHE:N	2:D:68:PHE:CD1	2.75	0.55
2:C:15:ARG:NE	2:C:126:HIS:ND1	2.43	0.55
2:D:68:PHE:N	2:D:68:PHE:HD1	2.04	0.54
1:A:288:THR:HB	4:A:2002:CLR:H263	1.90	0.54
1:B:97:TYR:HB3	1:B:152:MET:HE2	1.89	0.53
1:B:236:VAL:O	1:B:240:LEU:HG	2.08	0.53
2:C:126:HIS:CD2	2:C:126:HIS:C	2.85	0.52
1:A:79:LEU:HD23	1:A:332:PHE:HZ	1.75	0.52
1:A:148:THR:HG22	1:A:152:MET:HE3	1.93	0.51
1:B:193:ALA:HA	1:B:212:LEU:HD21	1.92	0.50
2:C:22:LEU:HD12	2:C:81:LEU:HD23	1.94	0.50
2:D:22:LEU:HD12	2:D:81:LEU:HD23	1.94	0.50
2:C:40:ALA:HB3	2:C:43:LYS:HB2	1.94	0.49
1:B:56:PRO:HB2	1:B:58:ILE:HG12	1.93	0.49
1:A:105:ASP:HA	1:A:108:VAL:HG22	1.93	0.49
1:A:143:PHE:CE1	1:A:234:ALA:HB2	2.48	0.49
2:D:6:LEU:HD22	2:D:24:CYS:SG	2.52	0.49
1:B:105:ASP:HA	1:B:108:VAL:HG22	1.93	0.49
1:A:193:ALA:HA	1:A:212:LEU:HD21	1.94	0.48
2:C:68:PHE:HD1	2:C:68:PHE:N	2.11	0.48
1:B:328:ILE:O	1:B:332:PHE:HB3	2.14	0.47
1:B:149:LEU:HD11	1:B:330:TYR:CE1	2.49	0.47
1:A:328:ILE:HA	1:A:332:PHE:HB2	1.96	0.47
1:B:111:THR:HB	3:B:2001:CVV:I1	2.85	0.47
2:C:68:PHE:N	2:C:68:PHE:CD1	2.81	0.47
1:A:56:PRO:HB2	1:A:58:ILE:HG13	1.97	0.47
2:C:44:GLU:HG3	2:C:45:ARG:H	1.80	0.47
1:B:235:PHE:O	1:B:239:VAL:HG23	2.14	0.46
1:A:232:ILE:HA	1:A:236:VAL:HB	1.96	0.46
1:A:134:VAL:CG1	3:A:2001:CVV:I1	3.34	0.46
2:C:68:PHE:CD2	2:C:83:MET:HG2	2.51	0.46
1:B:134:VAL:CG1	3:B:2001:CVV:I1	3.35	0.45
1:B:142:MET:HE3	1:B:287:TRP:CZ3	2.51	0.45
1:A:176:LYS:O	1:A:180:ILE:HG13	2.16	0.44
1:B:224:LEU:O	1:B:228:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:MET:HE3	1:A:287:TRP:CZ3	2.52	0.43
2:D:93:VAL:HA	2:D:119:GLN:HA	2.00	0.43
1:A:69:VAL:CB	1:A:112:MET:HE1	2.47	0.43
2:C:44:GLU:HG3	2:C:45:ARG:N	2.34	0.43
2:D:97:ALA:HB1	2:D:111:TYR:HB3	2.01	0.43
2:C:87:LYS:HE3	2:C:89:GLU:HB2	1.99	0.43
1:A:79:LEU:HD23	1:A:332:PHE:CZ	2.54	0.42
1:A:237:ILE:N	1:A:238:PRO:CD	2.82	0.42
2:D:68:PHE:CD2	2:D:83:MET:HG2	2.54	0.42
2:C:22:LEU:HB2	2:C:81:LEU:HB3	2.00	0.42
1:B:220:SER:HA	1:B:222:TRP:CZ3	2.55	0.42
1:B:292:ILE:HG22	4:B:2002:CLR:H72	2.01	0.42
2:D:22:LEU:HB2	2:D:81:LEU:HB3	2.00	0.42
1:B:66:TYR:HA	1:B:112:MET:HE2	2.02	0.41
1:B:232:ILE:HA	1:B:236:VAL:HB	2.03	0.41
1:A:104:ALA:HA	1:A:141:ASN:HD22	1.84	0.41
1:A:329:LEU:HA	1:A:333:LEU:HD12	2.02	0.41
1:A:108:VAL:HG13	1:A:141:ASN:HB3	2.03	0.41
2:C:68:PHE:CE2	2:C:83:MET:SD	3.14	0.41
1:A:292:ILE:HG22	4:A:2002:CLR:H72	2.02	0.40
1:B:160:VAL:HG12	1:B:252:ARG:HG2	2.04	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	273/418 (65%)	257 (94%)	16 (6%)	0	100	100
1	B	261/418 (62%)	249 (95%)	12 (5%)	0	100	100
2	C	124/134 (92%)	116 (94%)	8 (6%)	0	100	100
2	D	118/134 (88%)	108 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	776/1104 (70%)	730 (94%)	46 (6%)	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	223/369 (60%)	222 (100%)	1 (0%)	84	86
1	B	209/369 (57%)	209 (100%)	0	100	100
2	C	100/112 (89%)	99 (99%)	1 (1%)	68	79
2	D	92/112 (82%)	88 (96%)	4 (4%)	26	57
All	All	624/962 (65%)	618 (99%)	6 (1%)	68	79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	HIS
2	C	126	HIS
2	D	68	PHE
2	D	88	HIS
2	D	110	ASP
2	D	126	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	322	ASN
1	B	179	ASN
1	B	213	GLN
2	C	5	GLN
2	C	125	HIS

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Mol	Chain	Res	Type
2	D	5	GLN
2	D	119	GLN
2	D	125	HIS

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 ⓘ

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	CLR	A	2002	-	31,31,31	0.67	0	48,48,48	1.53	10 (20%)
4	CLR	B	2002	-	31,31,31	0.69	0	48,48,48	1.53	10 (20%)
3	CVV	A	2001	-	38,39,39	1.30	5 (13%)	58,61,61	1.31	7 (12%)
5	OLA	A	2003	-	13,13,19	0.76	0	13,13,19	1.06	1 (7%)
3	CVV	B	2001	-	38,39,39	1.31	5 (13%)	58,61,61	1.32	8 (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
4	CLR	A	2002	-	-	6/10/68/68	0/4/4/4
4	CLR	B	2002	-	-	5/10/68/68	0/4/4/4
3	CVV	A	2001	-	-	2/12/63/63	0/8/7/7
5	OLA	A	2003	-	-	6/11/11/17	-
3	CVV	B	2001	-	-	2/12/63/63	0/8/7/7

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	CVV	C10-C9	-4.31	1.40	1.50
3	B	2001	CVV	C10-C9	-4.06	1.41	1.50
3	A	2001	CVV	C20-C19	-2.74	1.34	1.40
3	B	2001	CVV	C8-N1	2.57	1.49	1.46
3	B	2001	CVV	C20-C19	-2.47	1.35	1.40
3	B	2001	CVV	C3-C4	2.46	1.59	1.54
3	A	2001	CVV	C3-C4	2.41	1.59	1.54
3	A	2001	CVV	C8-N1	2.37	1.49	1.46
3	A	2001	CVV	C19-C18	-2.30	1.34	1.38
3	B	2001	CVV	C19-C18	-2.11	1.35	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2002	CLR	C4-C5-C10	4.15	121.73	116.42
4	A	2002	CLR	C4-C5-C10	4.00	121.54	116.42
3	B	2001	CVV	C20-C19-C18	-3.36	116.88	120.97
4	B	2002	CLR	C4-C5-C6	-3.30	116.10	120.57
4	A	2002	CLR	C4-C5-C6	-3.23	116.19	120.57
3	A	2001	CVV	C21-C1-C2	-3.22	117.19	121.39
3	B	2001	CVV	C21-C1-C2	-3.19	117.22	121.39
3	A	2001	CVV	C3-C4-N2	-3.17	110.24	115.77
3	A	2001	CVV	C20-C19-C18	-3.14	117.14	120.97
4	A	2002	CLR	C12-C11-C9	3.05	118.32	113.14
4	B	2002	CLR	C12-C11-C9	3.05	118.32	113.14
3	B	2001	CVV	C3-C4-N2	-2.95	110.62	115.77
3	B	2001	CVV	C22-C17-C16	-2.89	109.13	111.68
3	B	2001	CVV	O3-C19-C20	2.82	131.06	126.14
3	A	2001	CVV	C22-C17-C16	-2.78	109.23	111.68
3	A	2001	CVV	O3-C19-C20	2.59	130.67	126.14
4	B	2002	CLR	C14-C8-C9	2.57	112.45	109.09
4	A	2002	CLR	C14-C8-C9	2.52	112.38	109.09
4	A	2002	CLR	C18-C13-C14	2.47	116.15	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2001	CVV	C17-C18-C2	-2.43	124.62	126.68
4	B	2002	CLR	C18-C13-C14	2.42	116.07	111.68
3	A	2001	CVV	C10-C11-C12	2.37	121.59	119.47
4	B	2002	CLR	C21-C20-C17	2.35	116.41	112.88
4	A	2002	CLR	C21-C20-C17	2.34	116.40	112.88
4	B	2002	CLR	C13-C17-C20	2.32	123.07	119.50
4	B	2002	CLR	C13-C14-C8	-2.29	111.16	114.41
3	B	2001	CVV	C10-C11-C12	2.29	121.51	119.47
4	A	2002	CLR	C13-C14-C8	-2.27	111.20	114.41
5	A	2003	OLA	O2-C1-C2	2.24	121.09	114.00
4	A	2002	CLR	C8-C7-C6	-2.19	109.73	112.76
4	B	2002	CLR	C8-C7-C6	-2.15	109.78	112.76
4	B	2002	CLR	C7-C8-C14	2.13	113.95	110.93
4	A	2002	CLR	C13-C17-C20	2.13	122.78	119.50
3	B	2001	CVV	C8-N1-C9	2.07	126.06	121.97
4	A	2002	CLR	C7-C8-C14	2.05	113.84	110.93
3	A	2001	CVV	C8-N1-C9	2.01	125.94	121.97

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2002	CLR	C17-C20-C22-C23
4	A	2002	CLR	C17-C20-C22-C23
4	A	2002	CLR	C20-C22-C23-C24
4	B	2002	CLR	C22-C23-C24-C25
4	B	2002	CLR	C21-C20-C22-C23
4	A	2002	CLR	C21-C20-C22-C23
4	B	2002	CLR	C23-C24-C25-C27
4	A	2002	CLR	C23-C24-C25-C27
4	A	2002	CLR	C23-C24-C25-C26
4	B	2002	CLR	C23-C24-C25-C26
5	A	2003	OLA	C5-C6-C7-C8
5	A	2003	OLA	C6-C7-C8-C9
4	A	2002	CLR	C22-C23-C24-C25
5	A	2003	OLA	C3-C4-C5-C6
3	A	2001	CVV	C7-C8-N1-C9
5	A	2003	OLA	O1-C1-C2-C3
5	A	2003	OLA	O2-C1-C2-C3
5	A	2003	OLA	C1-C2-C3-C4
3	A	2001	CVV	C16-C8-N1-C9
3	B	2001	CVV	C16-C8-N1-C9

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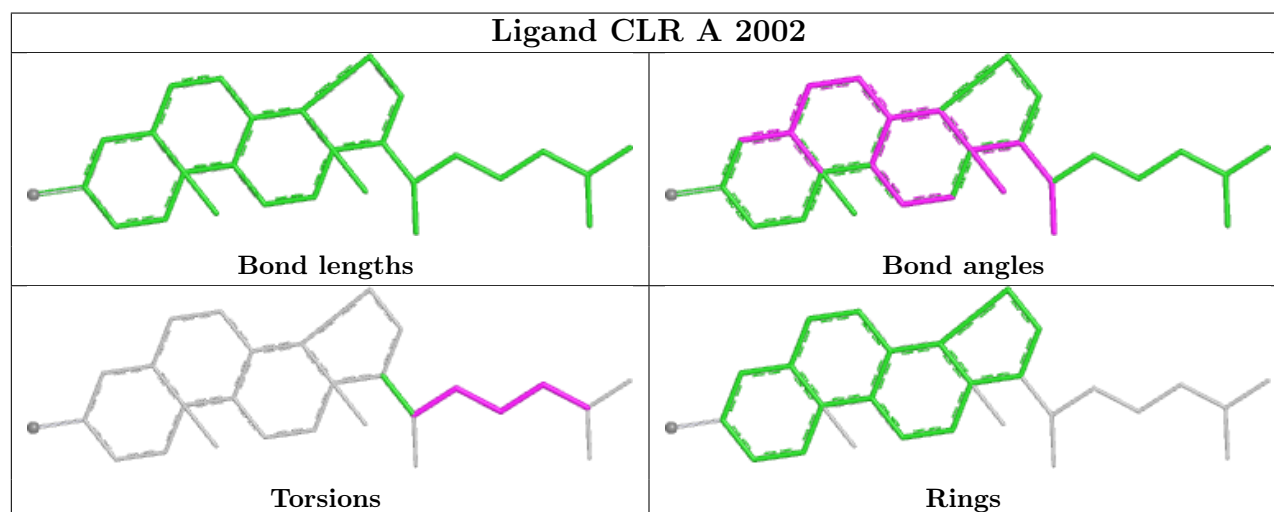
Mol	Chain	Res	Type	Atoms
3	B	2001	CVV	C7-C8-N1-C9

There are no ring outliers.

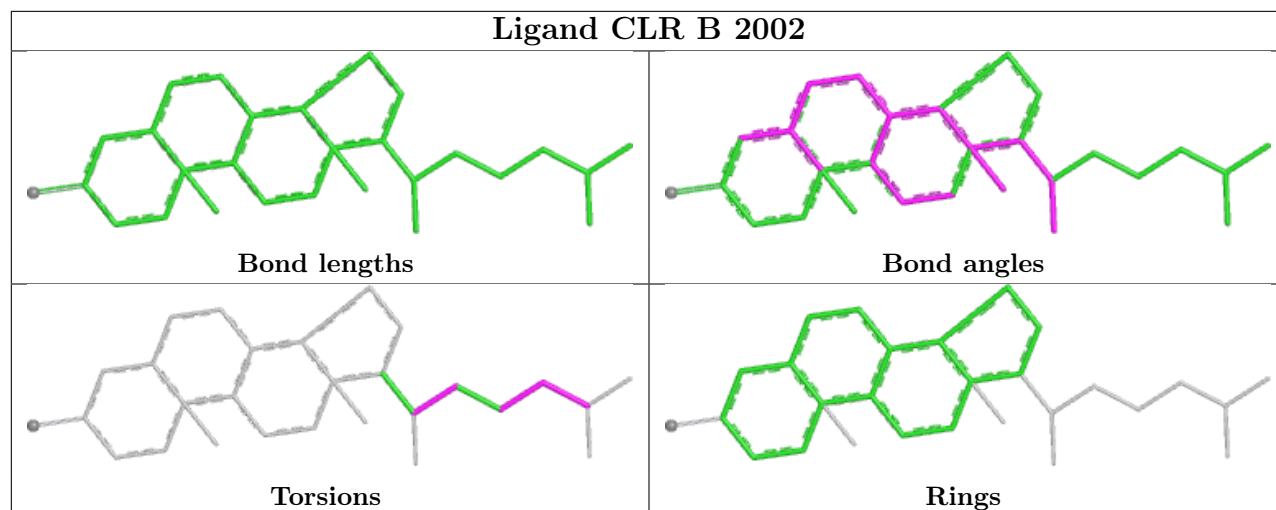
4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2002	CLR	3	0
4	B	2002	CLR	1	0
3	A	2001	CVV	2	0
3	B	2001	CVV	3	0

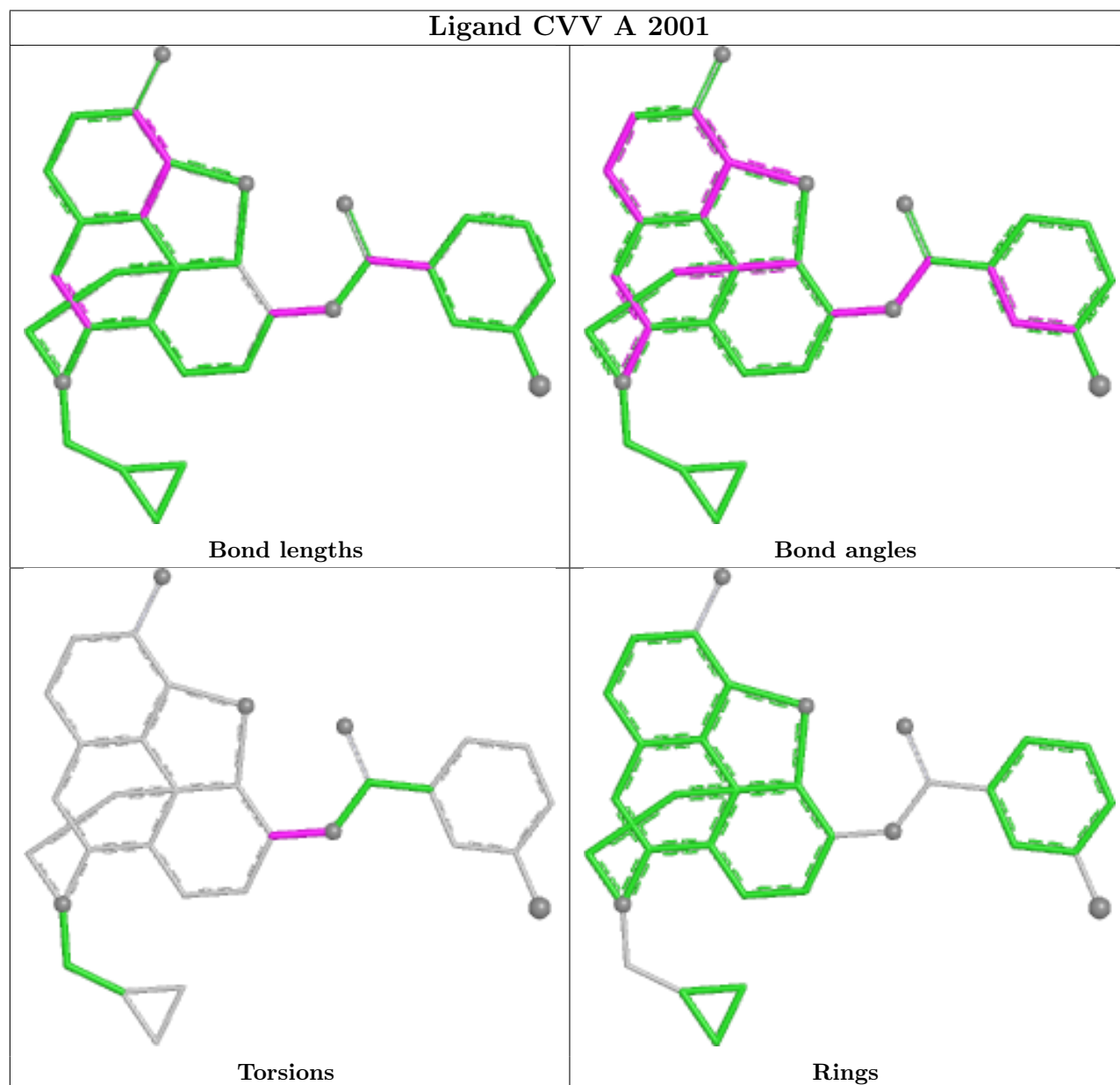
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

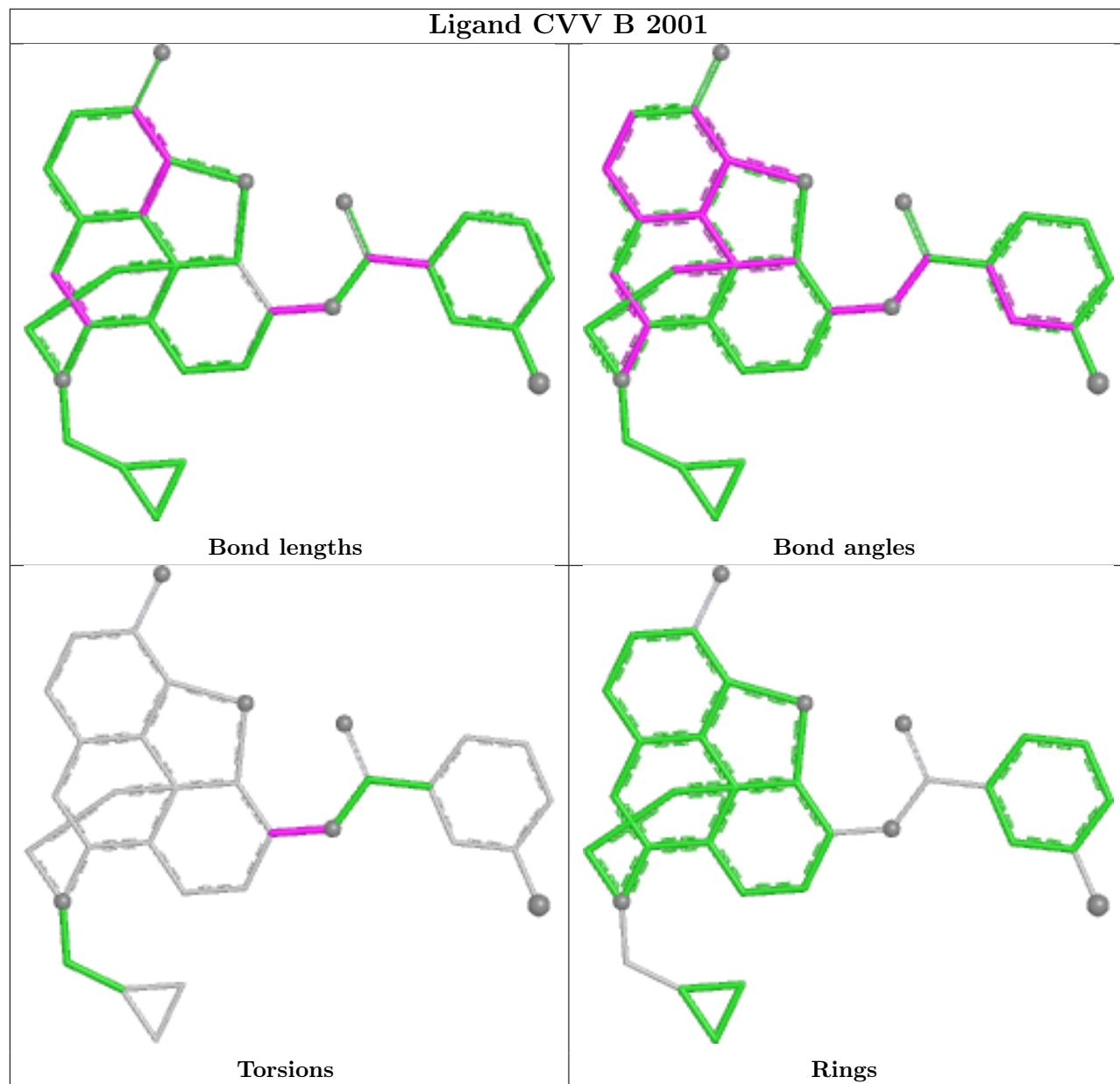
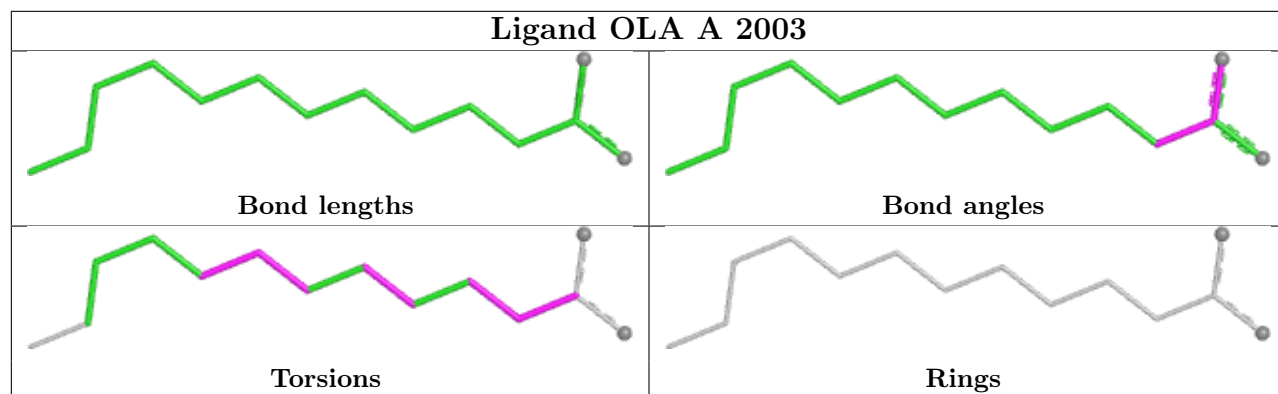


Ligand CLR B 2002



Ligand CVV A 2001





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	281/418 (67%)	0.89	33 (11%) 9 5	63, 78, 121, 146	0
1	B	269/418 (64%)	0.96	38 (14%) 6 3	61, 80, 113, 136	0
2	C	126/134 (94%)	1.23	22 (17%) 4 2	66, 84, 138, 169	0
2	D	122/134 (91%)	1.15	25 (20%) 2 1	66, 85, 122, 154	0
All	All	798/1104 (72%)	1.01	118 (14%) 5 3	61, 81, 122, 169	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	SER	6.3
2	C	32	TYR	6.1
2	D	129	HIS	5.5
1	B	306	THR	5.1
1	B	334	ASP	4.9
2	D	32	TYR	4.9
2	D	124	SER	4.8
1	B	269	LEU	4.7
1	B	266	ASP	4.5
2	C	76	ASN	4.2
1	B	216	ASP	4.1
2	D	109	TYR	3.9
1	B	305	SER	3.9
2	D	54	SER	3.9
2	C	125	HIS	3.9
1	B	219	TYR	3.8
1	B	78	SER	3.8
1	A	262	SER	3.8
2	D	125	HIS	3.8
1	B	181	CYS	3.8
1	A	132	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	333	LEU	3.7
2	D	4	VAL	3.7
2	D	127	HIS	3.6
2	C	54	SER	3.6
2	D	126	HIS	3.5
2	C	95	TYR	3.5
1	B	222	TRP	3.5
1	A	266	ASP	3.4
1	B	183	TRP	3.4
2	C	109	TYR	3.4
2	D	74	VAL	3.4
2	D	55	GLY	3.4
1	B	264	GLU	3.4
2	C	111	TYR	3.3
2	D	128	HIS	3.3
2	D	28	GLU	3.3
1	B	253	LEU	3.2
2	D	101	PRO	3.2
1	A	111	THR	3.2
1	A	336	ASN	3.2
1	B	217	ASP	3.1
2	C	4	VAL	3.1
1	A	269	LEU	3.1
2	C	103	GLY	3.1
1	A	332	PHE	3.1
2	D	102	VAL	3.1
1	A	127	GLY	3.0
2	D	114	TRP	3.0
1	A	257	ARG	3.0
1	B	258	LEU	2.9
1	A	87	TYR	2.9
2	C	53	TRP	2.9
2	C	84	ASN	2.8
1	B	332	PHE	2.8
1	A	334	ASP	2.8
2	D	53	TRP	2.8
1	B	185	LEU	2.7
2	C	129	HIS	2.7
1	A	186	SER	2.7
2	D	118	THR	2.6
1	A	338	LYS	2.6
1	B	106	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	305	SER	2.6
1	B	90	MET	2.6
2	C	127	HIS	2.6
1	B	91	LYS	2.6
2	D	95	TYR	2.5
1	B	215	PRO	2.5
1	A	248	LEU	2.5
2	D	111	TYR	2.5
1	B	188	SER	2.5
1	A	168	ASP	2.5
1	A	222	TRP	2.5
1	B	265	LYS	2.5
1	B	218	ASP	2.4
2	D	29	ARG	2.4
1	B	323	SER	2.4
2	C	101	PRO	2.4
2	C	126	HIS	2.4
1	A	339	ARG	2.4
2	D	107	SER	2.4
1	B	268	ASN	2.4
1	B	87	TYR	2.4
1	B	98	ILE	2.4
1	A	337	PHE	2.3
1	B	330	TYR	2.3
2	C	124	SER	2.3
2	C	60	TYR	2.3
1	A	335	GLU	2.3
1	B	95	ASN	2.3
2	C	57	ASP	2.3
2	C	108	PRO	2.2
1	A	194	ILE	2.2
1	B	226	MET	2.2
1	B	214	PHE	2.2
1	B	115	GLN	2.2
1	B	322	ASN	2.2
1	B	212	LEU	2.2
1	A	56	PRO	2.2
2	C	128	HIS	2.2
1	A	303	SER	2.2
1	A	323	SER	2.2
1	A	185	LEU	2.1
2	C	123	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	110	ASP	2.1
1	A	128	ASP	2.1
1	A	221	TRP	2.1
2	D	34	MET	2.1
2	D	40	ALA	2.1
1	A	264	GLU	2.1
1	A	82	PHE	2.1
1	A	302	THR	2.1
2	C	113	TYR	2.1
1	A	299	LEU	2.0
1	A	300	GLY	2.0
1	B	77	ASN	2.0
1	B	162	HIS	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](#)

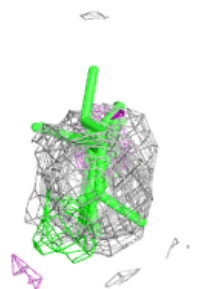
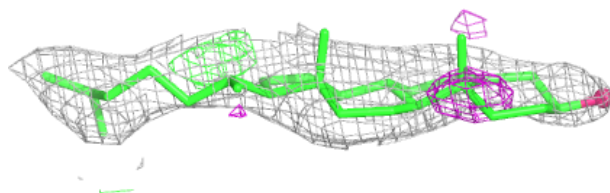
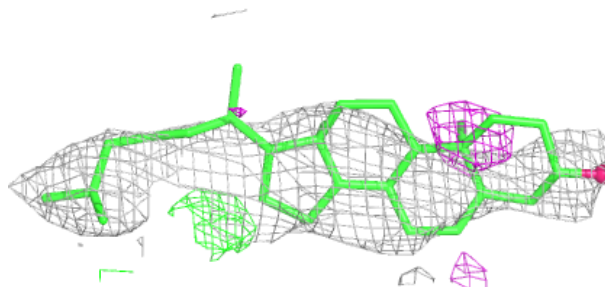
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	CLR	B	2002	28/28	0.69	0.32	111,122,123,124	0
4	CLR	A	2002	28/28	0.76	0.28	126,133,134,135	0
5	OLA	A	2003	14/20	0.90	0.16	61,74,86,86	0
3	CVV	B	2001	33/33	0.96	0.14	69,81,93,98	0
3	CVV	A	2001	33/33	0.96	0.13	66,77,93,98	0

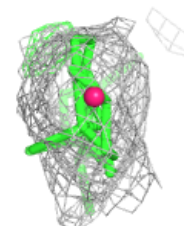
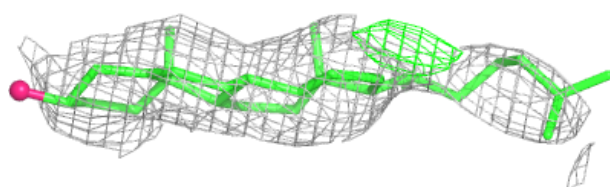
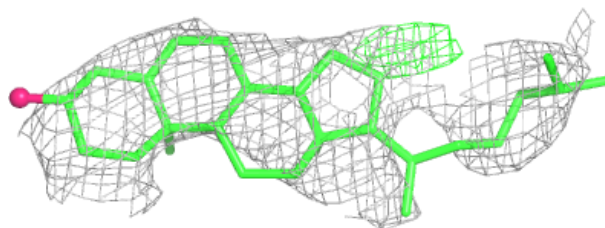
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CLR B 2002:

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

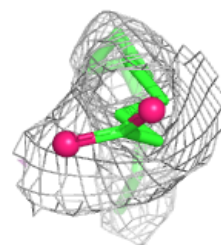
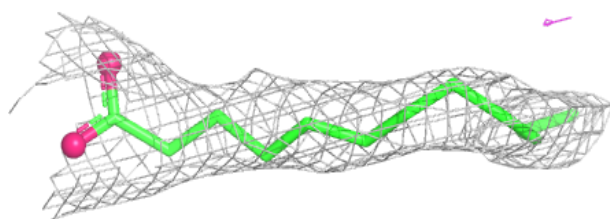
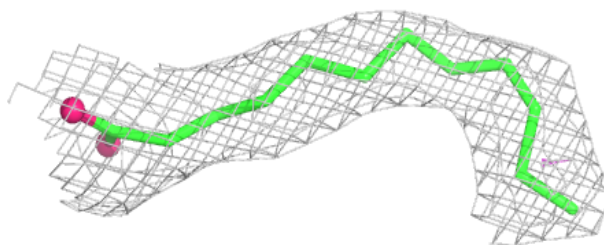
**Electron density around CLR A 2002:**

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



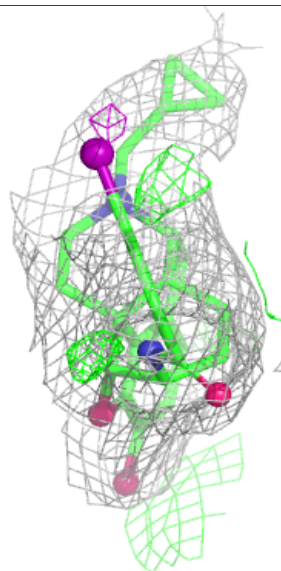
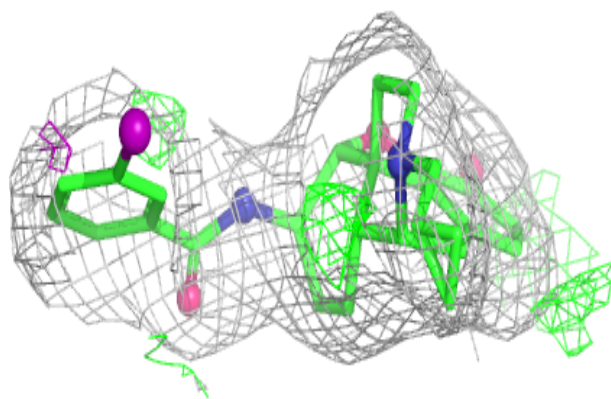
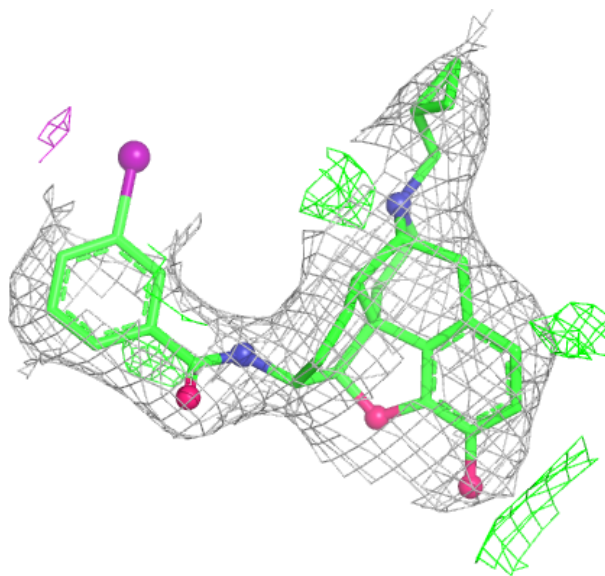
Electron density around OLA A 2003:

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



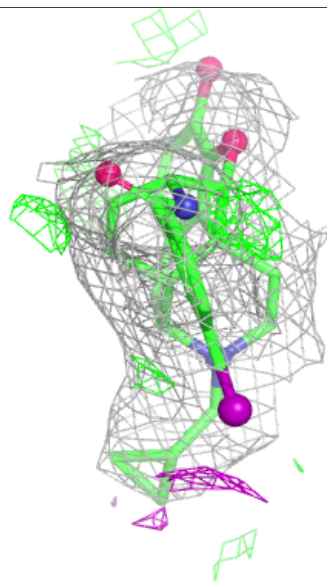
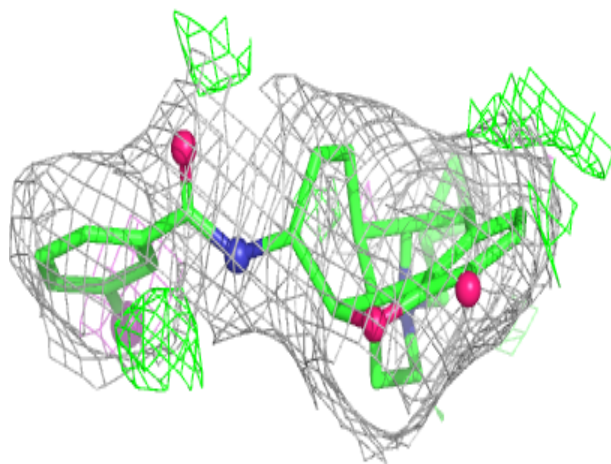
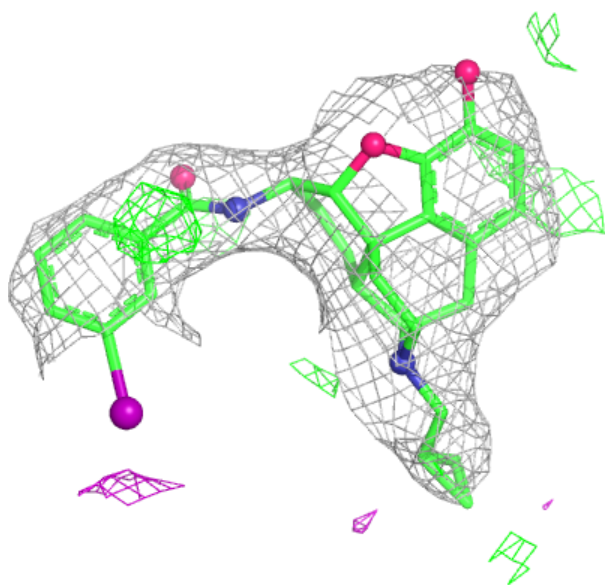
Electron density around CVV B 2001:

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



Electron density around CVV A 2001:

$2mF_o-DF_c$ (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.