



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:04 AM UTC

PDB ID : 6H7J / pdb_00006h7j
Title : ACTIVATED TURKEY BETA1 ADRENOCEPTOR WITH BOUND AGONIST ISOPRENALINE AND NANOBODY Nb80
Authors : Warne, T.; Edwards, P.C.; Dore, A.S.; Leslie, A.G.W.; Tate, C.G.
Deposited on : 2018-07-31
Resolution : 2.80 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

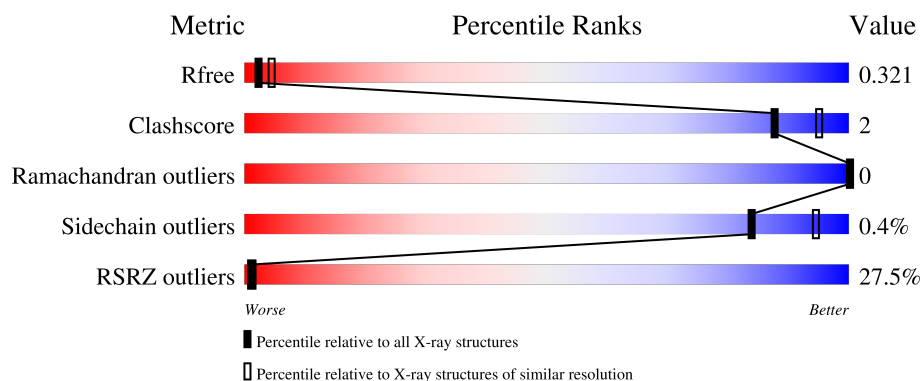
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	E	109	60% 97%
1	F	109	57% 94%
2	A	307	19% 88% 7% 6%
2	B	307	21% 84% 7% 9%
3	C	121	13% 96%

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Mol	Chain	Length	Quality of chain
3	D	121	15% 96% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8094 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	E	106	Total	C	N	O	0	0	0
			788	507	126	155			
1	F	106	Total	C	N	O	0	0	0
			801	517	127	157			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	32	SER	CYS	engineered mutation	UNP P0AA25
E	35	SER	CYS	engineered mutation	UNP P0AA25
E	109	GLU	-	expression tag	UNP P0AA25
F	32	SER	CYS	engineered mutation	UNP P0AA25
F	35	SER	CYS	engineered mutation	UNP P0AA25
F	109	GLU	-	expression tag	UNP P0AA25

- Molecule 2 is a protein called Beta-1 adrenergic receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	290	Total	C	N	O	S	0	0	0
			2308	1523	384	381	20			
2	B	280	Total	C	N	O	S	0	0	0
			2226	1478	363	366	19			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	ALA	-	expression tag	UNP P07700
A	40	ALA	-	expression tag	UNP P07700
A	41	ALA	-	expression tag	UNP P07700
A	42	LYS	-	expression tag	UNP P07700
A	43	VAL	-	expression tag	UNP P07700
A	68	SER	ARG	engineered mutation	UNP P07700

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Chain	Residue	Modelled	Actual	Comment	Reference
A	90	VAL	MET	engineered mutation	UNP P07700
A	116	LEU	CYS	engineered mutation	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
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	conflict	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	39	ALA	-	expression tag	UNP P07700
B	40	ALA	-	expression tag	UNP P07700
B	41	ALA	-	expression tag	UNP P07700

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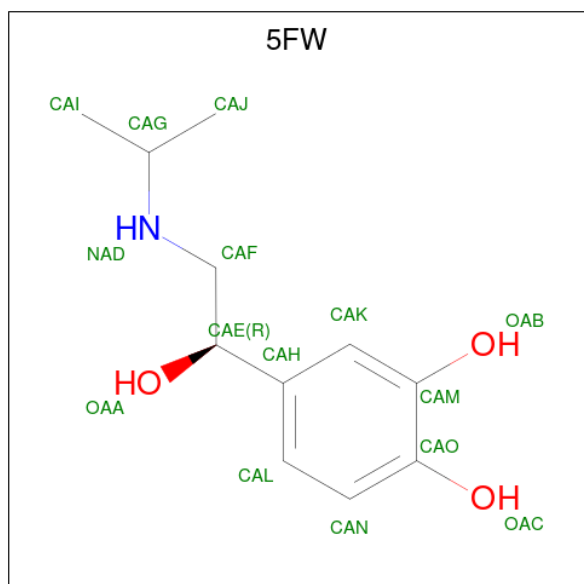
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Chain	Residue	Modelled	Actual	Comment	Reference
B	42	LYS	-	expression tag	UNP P07700
B	43	VAL	-	expression tag	UNP P07700
B	68	SER	ARG	engineered mutation	UNP P07700
B	90	VAL	MET	engineered mutation	UNP P07700
B	116	LEU	CYS	engineered mutation	UNP P07700
B	?	-	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
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	conflict	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 3 is a protein called Camelid antibody fragment Nb80.

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

- Molecule 4 is ISOPRENALINE (CCD ID: 5FW) (formula: $C_{11}H_{17}NO_3$).

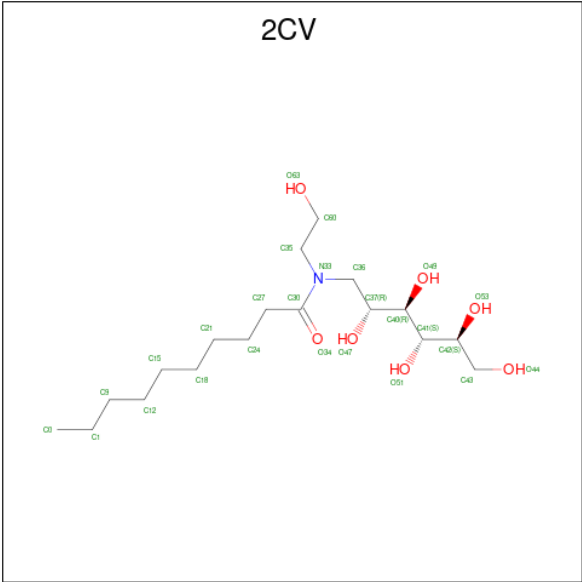


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	11	1	3		
4	B	1	Total	C	N	O	0	0
			15	11	1	3		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is HEGA-10 (CCD ID: 2CV) (formula: $C_{18}H_{37}NO_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			26	18	1	7		
6	A	1	Total	C	N	O	0	0
			16	14	1	1		
6	A	1	Total	C	N	O	0	0
			21	16	1	4		
6	B	1	Total	C	N	O	0	0
			26	18	1	7		
6	B	1	Total	C	N	O	0	0
			19	15	1	3		

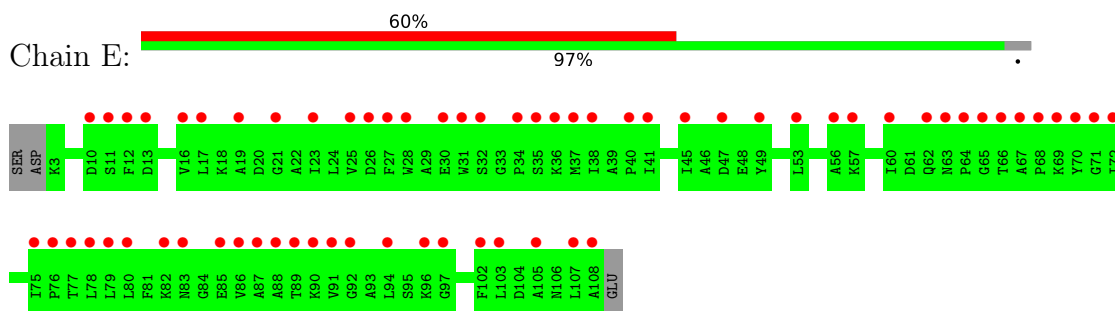
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total	O	0	0
			5	5		
7	C	5	Total	O	0	0
			5	5		
7	B	5	Total	O	0	0
			5	5		
7	D	5	Total	O	0	0
			5	5		

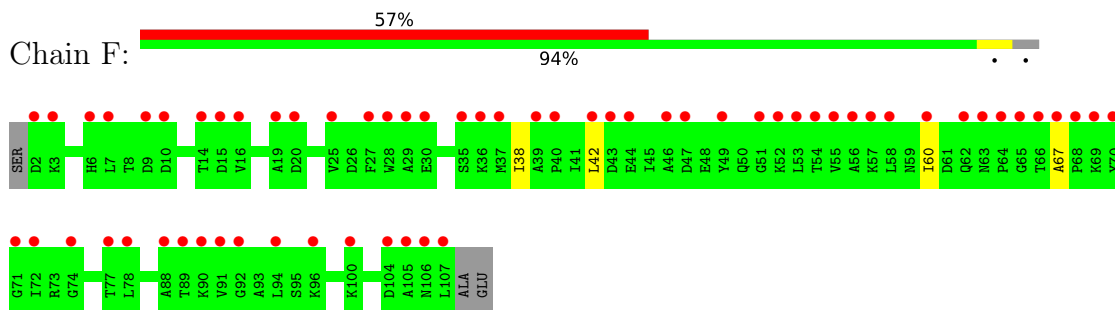
3 Residue-property plots

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.

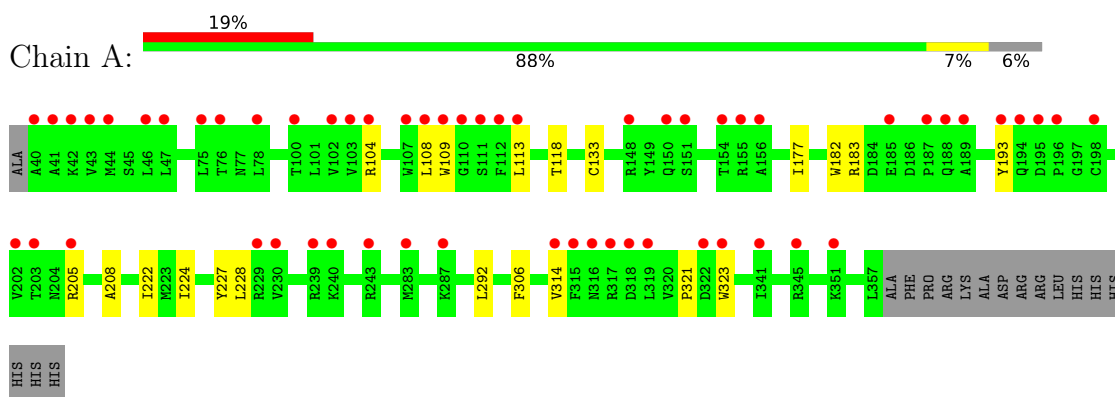
- Molecule 1: Thioredoxin 1



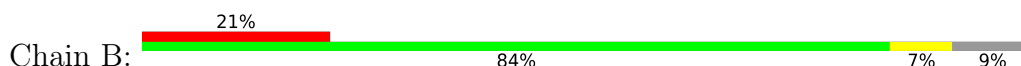
- Molecule 1: Thioredoxin 1

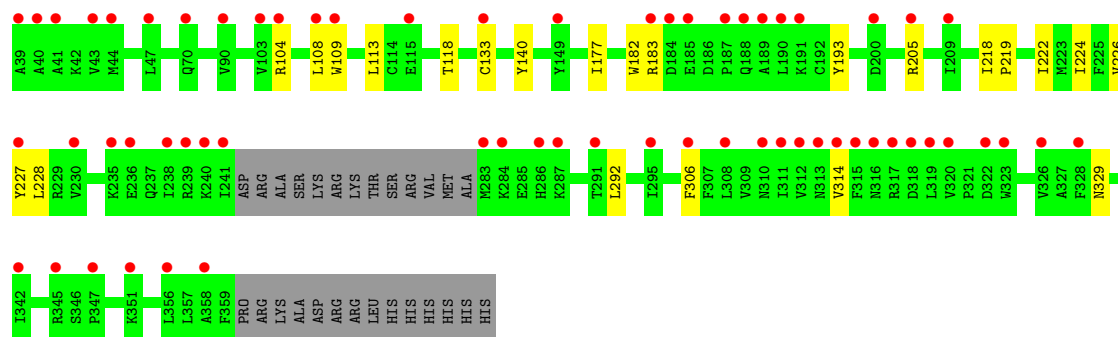


- Molecule 2: Beta-1 adrenergic receptor

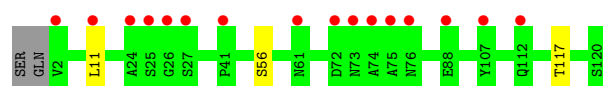


- Molecule 2: Beta-1 adrenergic receptor

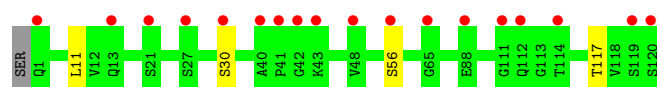




● Molecule 3: Camelid antibody fragment Nb80



● Molecule 3: 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	116.73Å 121.18Å 129.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.38 – 2.80 41.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	64.9 (41.38-2.80) 64.9 (41.38-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0174	Depositor
R, R_{free}	0.285 , 0.317 0.289 , 0.321	Depositor DCC
R_{free} test set	1439 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	8094	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 2CV, 5FW

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	E	0.67	0/803	0.77	0/1096
1	F	0.66	0/816	0.77	0/1109
2	A	0.61	0/2362	0.88	0/3215
2	B	0.62	0/2280	0.87	0/3107
3	C	0.53	0/918	0.63	0/1244
3	D	0.55	0/927	0.63	0/1256
All	All	0.61	0/8106	0.80	0/11027

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	E	788	0	770	0	0
1	F	801	0	802	2	0
2	A	2308	0	2418	12	0
2	B	2226	0	2322	13	0
3	C	901	0	861	1	0
3	D	910	0	872	1	0
4	A	15	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	15	0	15	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	63	0	90	2	0
6	B	45	0	62	1	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
All	All	8094	0	8227	32	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (32) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:TYR:HB3	2:B:292:LEU:HD11	1.77	0.67
2:A:227:TYR:HB3	2:A:292:LEU:HD11	1.76	0.66
2:A:104:ARG:HG3	2:A:108:LEU:HD11	1.92	0.50
2:B:183:ARG:HD2	2:B:193:TYR:CD2	2.46	0.50
2:B:140:TYR:HB2	2:B:226:VAL:HG13	1.94	0.49
3:D:11:LEU:HD23	3:D:117:THR:HB	1.93	0.49
1:F:38:ILE:HD12	1:F:42:LEU:HD11	1.94	0.49
3:C:11:LEU:HD23	3:C:117:THR:HB	1.94	0.48
6:A:403:2CV:O34	6:A:403:2CV:O47	2.31	0.48
2:B:306:PHE:CZ	4:B:402:5FW:HAE	2.49	0.47
2:A:306:PHE:CZ	4:A:401:5FW:HAE	2.49	0.47
2:A:183:ARG:HD2	2:A:193:TYR:CD2	2.49	0.47
2:B:109:TRP:HB3	2:B:113:LEU:HD12	1.98	0.45
2:A:109:TRP:HB3	2:A:113:LEU:HD12	1.98	0.45
2:A:118:THR:HG22	2:A:177:ILE:HD13	1.99	0.45
2:B:177:ILE:HA	2:B:182:TRP:CD1	2.52	0.45
2:A:321:PRO:HB2	2:A:323:TRP:CD1	2.52	0.44
2:B:104:ARG:HG3	2:B:108:LEU:HD11	1.98	0.44
2:B:118:THR:HG22	2:B:177:ILE:HD13	1.99	0.44
2:A:133:CYS:SG	2:A:222:ILE:HB	2.57	0.44
2:A:177:ILE:HA	2:A:182:TRP:CD1	2.52	0.44
2:B:329:ASN:C	2:B:329:ASN:HD22	2.24	0.44
2:A:224:ILE:O	2:A:228:LEU:HB2	2.18	0.44
2:B:224:ILE:O	2:B:228:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ARG:HG3	2:B:314:VAL:HG11	2.00	0.42
2:A:208:ALA:HB3	2:A:314:VAL:HG21	2.02	0.41
2:A:205:ARG:HG3	2:A:314:VAL:HG11	2.03	0.41
6:B:401:2CV:H362	6:B:401:2CV:O51	2.20	0.41
2:B:133:CYS:SG	2:B:222:ILE:HB	2.60	0.41
2:B:218:ILE:HB	2:B:219:PRO:HD3	2.02	0.41
6:A:403:2CV:H40	6:A:403:2CV:O63	2.22	0.40
1:F:60:ILE:HD12	1:F:67:ALA:HB2	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	E	104/109 (95%)	103 (99%)	1 (1%)	0	100	100
1	F	104/109 (95%)	103 (99%)	1 (1%)	0	100	100
2	A	288/307 (94%)	279 (97%)	9 (3%)	0	100	100
2	B	276/307 (90%)	268 (97%)	8 (3%)	0	100	100
3	C	117/121 (97%)	114 (97%)	3 (3%)	0	100	100
3	D	118/121 (98%)	115 (98%)	3 (2%)	0	100	100
All	All	1007/1074 (94%)	982 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	80/88 (91%)	80 (100%)	0	100	100
1	F	84/88 (96%)	84 (100%)	0	100	100
2	A	252/266 (95%)	252 (100%)	0	100	100
2	B	242/266 (91%)	242 (100%)	0	100	100
3	C	94/96 (98%)	93 (99%)	1 (1%)	65	87
3	D	95/96 (99%)	93 (98%)	2 (2%)	47	79
All	All	847/900 (94%)	844 (100%)	3 (0%)	84	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	56	SER
3	D	30	SER
3	D	56	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	335	ASN
3	C	61	ASN
3	C	96	ASN
1	F	98	GLN
3	D	96	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 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
4	5FW	A	401	-	15,15,15	0.68	0	19,20,20	0.59	0
6	2CV	A	405	-	20,20,25	0.50	0	22,23,30	1.35	3 (13%)
4	5FW	B	402	-	15,15,15	0.59	0	19,20,20	0.55	0
6	2CV	A	403	-	25,25,25	0.43	0	29,30,30	1.48	6 (20%)
6	2CV	A	404	-	15,15,25	0.53	0	16,16,30	1.21	2 (12%)
6	2CV	B	404	-	18,18,25	0.52	0	20,21,30	0.96	1 (5%)
6	2CV	B	401	-	25,25,25	0.43	0	29,30,30	1.68	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
4	5FW	A	401	-	-	0/9/9/9	0/1/1/1
6	2CV	A	405	-	-	4/24/24/34	-
4	5FW	B	402	-	-	0/9/9/9	0/1/1/1
6	2CV	A	403	-	-	8/34/34/34	-
6	2CV	A	404	-	-	4/17/17/34	-
6	2CV	B	404	-	-	8/21/21/34	-
6	2CV	B	401	-	-	12/34/34/34	-

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	401	2CV	C43-C42-C41	4.75	121.84	112.17
6	A	405	2CV	C27-C30-N33	3.80	123.85	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	405	2CV	C60-C35-N33	-3.39	104.75	112.66
6	B	401	2CV	C42-C41-C40	3.36	117.64	112.48
6	A	403	2CV	C36-C37-C40	3.08	118.02	109.66
6	A	403	2CV	C24-C27-C30	-3.06	104.73	112.66
6	A	404	2CV	C27-C30-N33	3.04	122.69	118.09
6	A	403	2CV	C37-C40-C41	-2.92	107.99	112.48
6	B	401	2CV	C27-C30-N33	2.70	122.18	118.09
6	B	401	2CV	C36-C37-C40	2.69	116.95	109.66
6	A	404	2CV	O34-C30-C27	-2.53	114.43	121.26
6	A	403	2CV	O34-C30-C27	-2.49	114.52	121.26
6	A	403	2CV	C27-C30-N33	2.28	121.55	118.09
6	A	405	2CV	O34-C30-C27	-2.05	115.71	121.26
6	B	404	2CV	C35-N33-C36	-2.01	114.47	116.87
6	A	403	2CV	O47-C37-C40	-2.00	104.57	109.25

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	401	2CV	N33-C36-C37-C40
6	B	401	2CV	N33-C36-C37-O47
6	B	404	2CV	N33-C36-C37-O47
6	B	401	2CV	C40-C41-C42-C43
6	A	403	2CV	O34-C30-N33-C36
6	B	401	2CV	C24-C27-C30-N33
6	B	401	2CV	C24-C27-C30-O34
6	A	403	2CV	C27-C30-N33-C36
6	A	405	2CV	N33-C35-C60-O63
6	B	401	2CV	O51-C41-C42-O53
6	B	401	2CV	N33-C35-C60-O63
6	B	404	2CV	C36-C37-C40-C41
6	A	405	2CV	C37-C36-N33-C35
6	A	404	2CV	C12-C15-C18-C21
6	B	404	2CV	O34-C30-N33-C35
6	A	403	2CV	C15-C18-C21-C24
6	B	401	2CV	C40-C41-C42-O53
6	B	401	2CV	O51-C41-C42-C43
6	A	404	2CV	C24-C27-C30-O34
6	A	405	2CV	C24-C27-C30-O34
6	A	405	2CV	C24-C27-C30-N33
6	B	404	2CV	C27-C30-N33-C36
6	A	403	2CV	O34-C30-N33-C35

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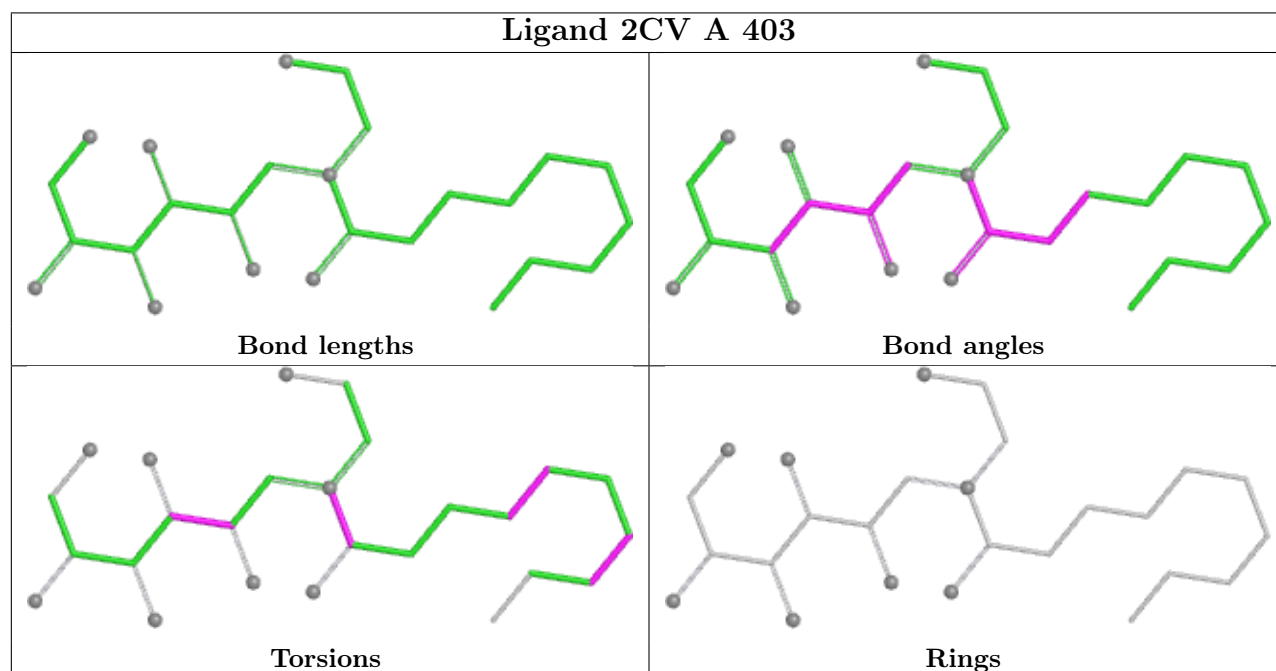
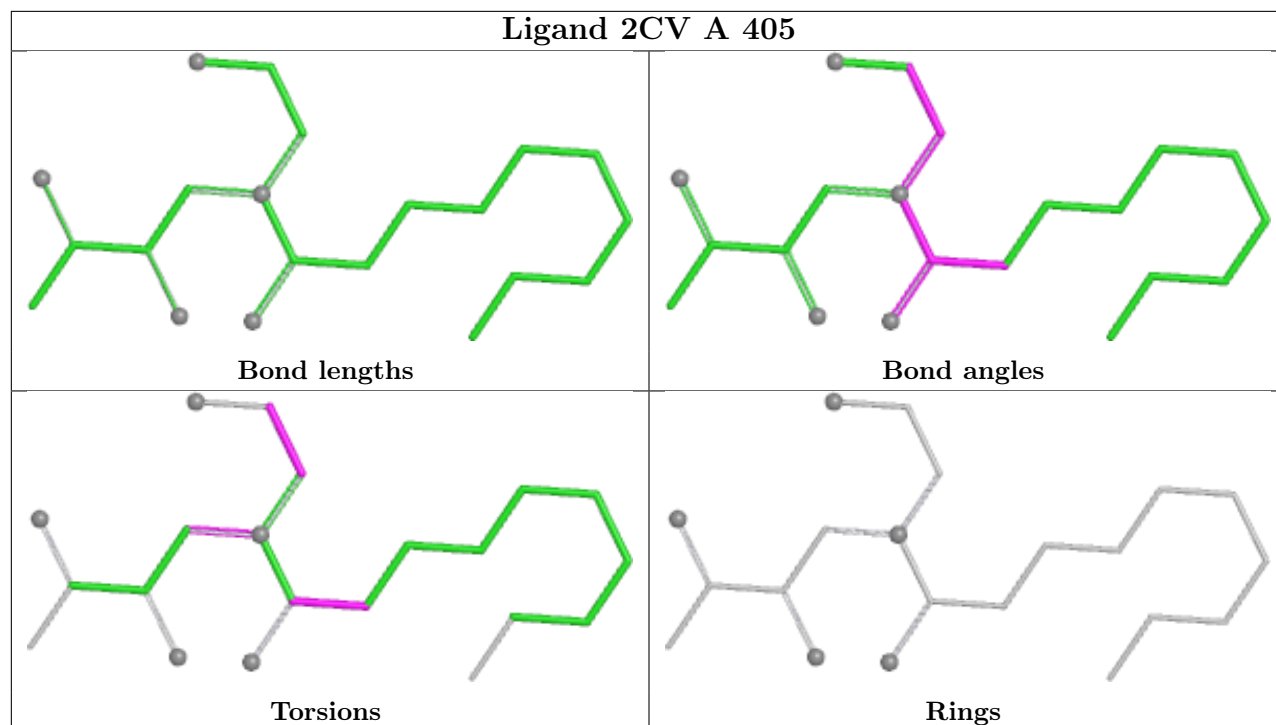
Mol	Chain	Res	Type	Atoms
6	B	404	2CV	C27-C30-N33-C35
6	A	403	2CV	C27-C30-N33-C35
6	B	404	2CV	C24-C27-C30-O34
6	A	404	2CV	C24-C27-C30-N33
6	B	401	2CV	C15-C18-C21-C24
6	A	403	2CV	C36-C37-C40-O49
6	B	401	2CV	C27-C30-N33-C36
6	A	403	2CV	C15-C12-C9-C1
6	B	401	2CV	O34-C30-N33-C36
6	B	404	2CV	N33-C36-C37-C40
6	A	404	2CV	C15-C12-C9-C1
6	B	404	2CV	C24-C27-C30-N33
6	A	403	2CV	O47-C37-C40-O49

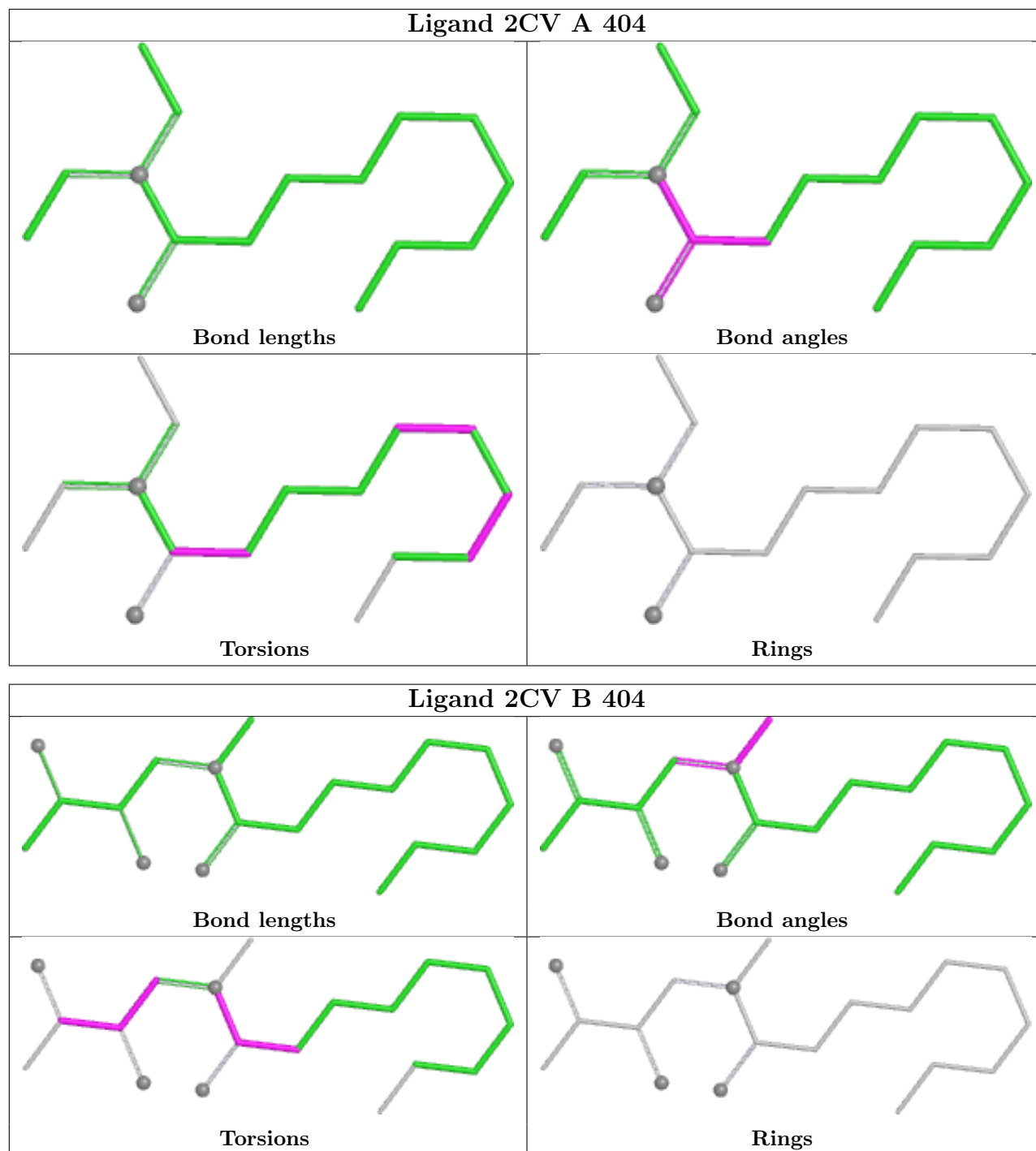
There are no ring outliers.

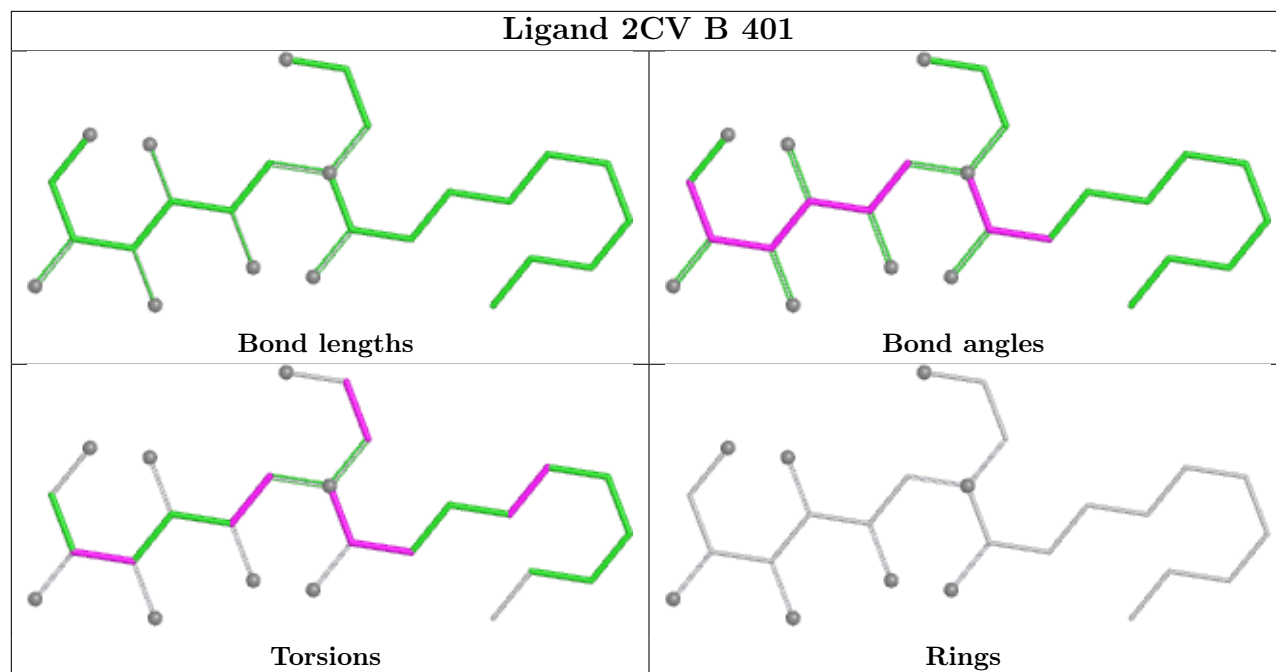
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	5FW	1	0
4	B	402	5FW	1	0
6	A	403	2CV	2	0
6	B	401	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.







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	E	106/109 (97%)	2.64	65 (61%) 0 0	73, 129, 189, 197	0
1	F	106/109 (97%)	2.32	62 (58%) 0 0	62, 112, 150, 178	0
2	A	290/307 (94%)	1.05	57 (19%) 3 2	22, 55, 102, 127	0
2	B	280/307 (91%)	1.47	63 (22%) 2 1	28, 61, 107, 137	0
3	C	119/121 (98%)	0.78	16 (13%) 7 5	25, 49, 88, 95	0
3	D	120/121 (99%)	1.06	18 (15%) 5 4	36, 60, 93, 117	0
All	All	1021/1074 (95%)	1.43	281 (27%) 1 1	22, 64, 140, 197	0

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	88	ALA	8.7
2	B	313	ASN	8.4
1	E	78	LEU	8.2
2	B	239	ARG	7.4
1	E	77	THR	7.0
2	B	188	GLN	6.8
1	E	89	THR	6.5
2	A	315	PHE	6.3
2	B	312	VAL	6.1
1	E	87	ALA	5.8
2	B	317	ARG	5.7
1	E	79	LEU	5.7
2	B	240	LYS	5.5
1	E	90	LYS	5.4
1	F	15	ASP	5.4
2	A	112	PHE	5.4
1	F	105	ALA	5.4
2	B	318	ASP	5.2
2	B	41	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
2	B	345	ARG	5.2
1	E	31	TRP	5.2
3	C	75	ALA	5.1
1	E	76	PRO	5.0
3	C	88	GLU	4.9
2	B	319	LEU	4.8
1	E	108	ALA	4.7
2	A	111	SER	4.7
1	F	68	PRO	4.7
2	A	317	ARG	4.6
3	D	1	GLN	4.5
1	E	26	ASP	4.4
1	E	80	LEU	4.4
2	B	43	VAL	4.4
1	F	28	TRP	4.3
1	E	105	ALA	4.3
1	F	94	LEU	4.3
1	E	13	ASP	4.3
1	E	67	ALA	4.3
2	B	310	ASN	4.2
2	B	316	ASN	4.2
1	F	14	THR	4.2
2	A	318	ASP	4.2
2	A	194	GLN	4.2
2	A	243	ARG	4.2
1	E	91	VAL	4.2
2	B	238	ILE	4.1
3	C	76	ASN	4.1
3	D	41	PRO	4.1
1	E	70	TYR	4.1
2	B	311	ILE	4.1
2	B	187	PRO	4.0
2	B	205	ARG	4.0
2	A	75	LEU	4.0
1	F	40	PRO	4.0
1	F	43	ASP	3.9
1	F	2	ASP	3.9
2	A	196	PRO	3.9
2	A	239	ARG	3.9
2	B	351	LYS	3.9
1	F	62	GLN	3.8
2	A	104	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	314	VAL	3.8
2	B	315	PHE	3.8
1	F	10	ASP	3.7
1	F	20	ASP	3.7
2	A	40	ALA	3.7
2	A	323	TRP	3.7
2	A	316	ASN	3.7
1	E	86	VAL	3.7
1	F	16	VAL	3.7
2	B	320	VAL	3.7
2	A	345	ARG	3.7
3	C	73	ASN	3.7
1	F	52	LYS	3.7
3	D	120	SER	3.6
3	C	72	ASP	3.6
2	A	41	ALA	3.6
3	C	74	ALA	3.6
1	E	23	ILE	3.6
1	F	72	ILE	3.6
3	C	25	SER	3.6
3	D	42	GLY	3.6
2	A	287	LYS	3.6
2	B	328	PHE	3.5
1	F	71	GLY	3.5
2	B	40	ALA	3.5
2	A	110	GLY	3.4
1	F	36	LYS	3.4
2	B	287	LYS	3.4
1	E	85	GLU	3.4
3	D	13	GLN	3.4
1	E	64	PRO	3.4
1	F	92	GLY	3.4
3	C	11	LEU	3.4
1	E	38	ILE	3.4
1	E	12	PHE	3.4
1	F	106	ASN	3.4
1	E	60	ILE	3.4
2	B	283	MET	3.4
2	B	356	LEU	3.3
1	E	34	PRO	3.3
2	B	291	THR	3.3
1	F	55	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	60	ILE	3.3
2	A	150	GLN	3.3
2	B	209	ILE	3.3
2	B	358	ALA	3.2
1	E	27	PHE	3.2
2	A	283	MET	3.2
1	E	94	LEU	3.2
2	A	151	SER	3.2
1	F	35	SER	3.2
3	D	119	SER	3.2
1	F	51	GLY	3.2
1	E	63	ASN	3.1
3	D	43	LYS	3.1
2	B	191	LYS	3.1
2	A	314	VAL	3.1
2	B	322	ASP	3.1
1	E	97	GLY	3.1
2	B	236	GLU	3.1
2	B	241	ILE	3.1
1	F	49	TYR	3.0
3	C	26	GLY	3.0
1	E	62	GLN	3.0
2	A	205	ARG	3.0
1	E	92	GLY	3.0
1	E	40	PRO	3.0
1	E	36	LYS	3.0
1	E	21	GLY	3.0
1	E	65	GLY	3.0
2	A	46	LEU	3.0
1	F	107	LEU	2.9
1	E	37	MET	2.9
1	E	25	VAL	2.9
2	B	189	ALA	2.9
2	A	108	LEU	2.9
2	B	109	TRP	2.9
1	F	70	TYR	2.9
2	A	185	GLU	2.9
1	E	45	ILE	2.9
2	A	44	MET	2.9
1	F	3	LYS	2.9
1	F	100	LYS	2.8
2	B	47	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	185	GLU	2.8
1	F	44	GLU	2.8
2	A	109	TRP	2.8
1	F	25	VAL	2.8
1	F	58	LEU	2.8
1	F	66	THR	2.8
2	B	184	ASP	2.8
2	A	148	ARG	2.7
2	A	103	VAL	2.7
2	A	202	VAL	2.7
3	D	48	VAL	2.7
2	A	240	LYS	2.7
2	A	155	ARG	2.7
2	A	42	LYS	2.7
1	F	54	THR	2.7
1	F	91	VAL	2.7
1	E	72	ILE	2.7
1	E	83	ASN	2.7
1	F	29	ALA	2.7
3	C	61	ASN	2.7
1	E	107	LEU	2.7
1	F	19	ALA	2.6
1	F	88	ALA	2.6
3	D	40	ALA	2.6
1	F	47	ASP	2.6
2	B	190	LEU	2.6
2	B	230	VAL	2.6
3	C	24	ALA	2.6
1	E	49	TYR	2.6
1	F	77	THR	2.6
1	F	63	ASN	2.6
1	F	96	LYS	2.6
1	F	64	PRO	2.6
2	A	319	LEU	2.6
2	B	108	LEU	2.6
1	E	41	ILE	2.6
2	B	115	GLU	2.6
1	F	27	PHE	2.6
1	F	67	ALA	2.6
2	B	200	ASP	2.6
2	B	104	ARG	2.5
1	E	57	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	A	188	GLN	2.5
3	D	114	THR	2.5
2	B	39	ALA	2.5
1	F	90	LYS	2.5
1	E	71	GLY	2.5
1	F	7	LEU	2.5
1	F	65	GLY	2.5
2	B	149	TYR	2.5
2	A	100	THR	2.5
2	B	183	ARG	2.5
1	F	104	ASP	2.5
3	C	27	SER	2.5
1	E	68	PRO	2.5
1	E	75	ILE	2.5
2	A	43	VAL	2.5
1	E	10	ASP	2.5
1	F	74	GLY	2.5
1	E	47	ASP	2.4
1	E	53	LEU	2.4
1	F	69	LYS	2.4
2	B	227	TYR	2.4
2	B	326	VAL	2.4
3	D	65	GLY	2.4
1	E	66	THR	2.4
1	F	37	MET	2.4
3	D	56	SER	2.4
1	E	28	TRP	2.4
1	E	96	LYS	2.4
2	A	113	LEU	2.3
2	A	187	PRO	2.3
2	A	230	VAL	2.3
1	E	11	SER	2.3
3	D	27	SER	2.3
3	C	107	TYR	2.3
2	B	235	LYS	2.3
1	E	16	VAL	2.3
1	F	30	GLU	2.3
3	D	112	GLN	2.3
2	B	286	HIS	2.3
2	A	154	THR	2.3
2	A	193	TYR	2.3
1	F	89	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	21	SER	2.3
1	F	56	ALA	2.2
1	E	69	LYS	2.2
1	F	57	LYS	2.2
2	A	195	ASP	2.2
3	D	111	GLY	2.2
1	E	30	GLU	2.2
3	D	88	GLU	2.2
2	A	341	ILE	2.2
3	C	112	GLN	2.2
1	F	9	ASP	2.2
2	B	323	TRP	2.2
3	C	2	VAL	2.2
1	E	19	ALA	2.2
2	B	90	VAL	2.2
2	B	347	PRO	2.2
2	A	203	THR	2.2
2	B	133	CYS	2.2
1	E	32	SER	2.2
1	F	42	LEU	2.2
1	F	39	ALA	2.2
1	F	6	HIS	2.2
2	B	103	VAL	2.2
3	C	41	PRO	2.2
2	A	107	TRP	2.2
2	B	306	PHE	2.2
3	D	30	SER	2.2
2	A	156	ALA	2.2
2	A	189	ALA	2.2
2	B	70	GLN	2.1
1	E	102	PHE	2.1
2	B	308	LEU	2.1
2	B	295	ILE	2.1
2	B	342	ILE	2.1
2	A	102	VAL	2.1
1	E	35	SER	2.1
1	E	103	LEU	2.1
2	A	78	LEU	2.1
2	A	322	ASP	2.1
2	A	229	ARG	2.1
2	A	351	LYS	2.0
1	E	17	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	53	LEU	2.0
1	F	78	LEU	2.0
2	A	76	THR	2.0
1	E	56	ALA	2.0
1	F	46	ALA	2.0
2	B	44	MET	2.0
2	A	198	CYS	2.0
2	A	47	LEU	2.0
1	E	82	LYS	2.0
2	B	284	LYS	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](#)

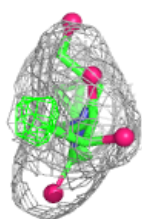
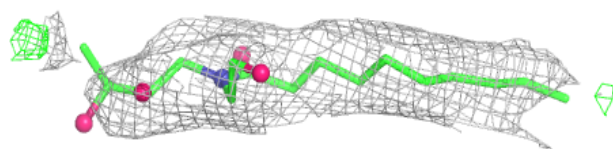
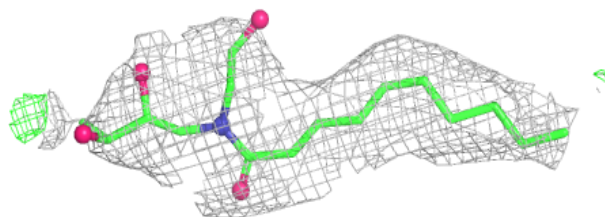
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NA	A	402	1/1	0.68	0.14	57,57,57,57	0
6	2CV	A	405	21/26	0.76	0.21	40,60,79,106	0
6	2CV	A	404	16/26	0.78	0.21	47,56,79,85	0
6	2CV	B	404	19/26	0.79	0.21	26,37,65,77	0
6	2CV	B	401	26/26	0.82	0.23	31,53,79,95	0
6	2CV	A	403	26/26	0.85	0.18	34,49,64,66	0
5	NA	B	403	1/1	0.90	0.15	47,47,47,47	0
4	5FW	B	402	15/15	0.92	0.12	44,57,61,61	0
4	5FW	A	401	15/15	0.92	0.12	41,47,61,68	0

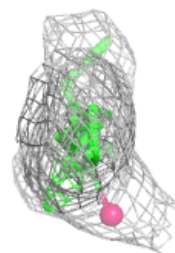
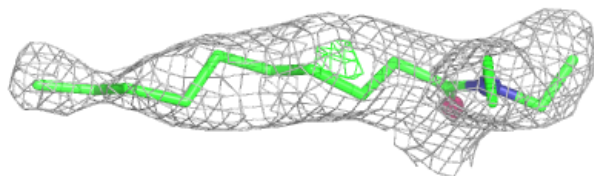
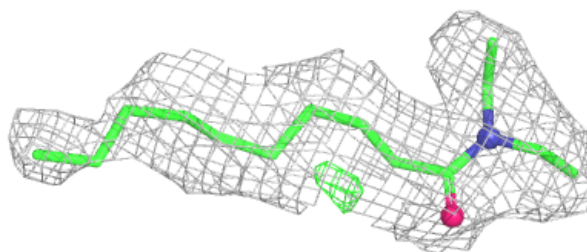
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2CV A 405:

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

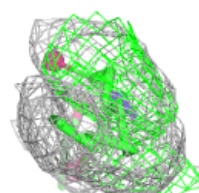
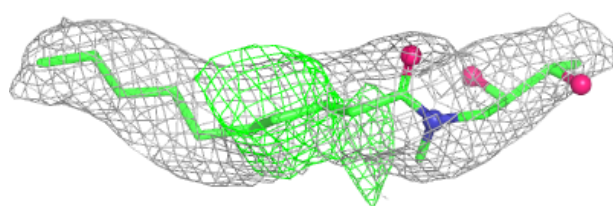
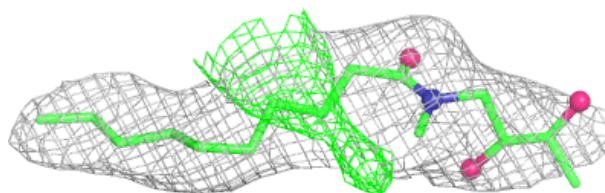
**Electron density around 2CV A 404:**

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

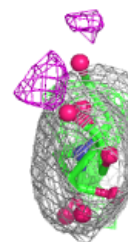
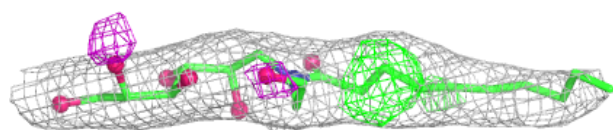
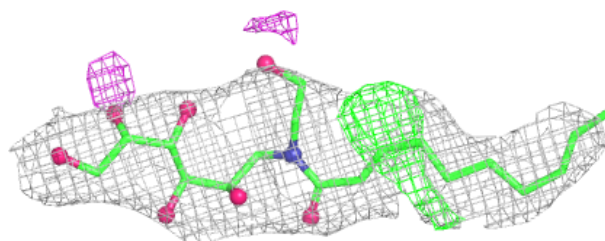


Electron density around 2CV B 404:

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

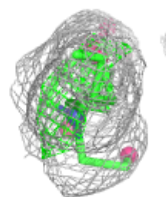
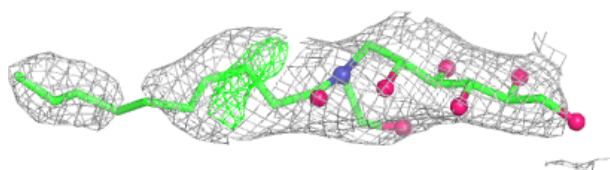
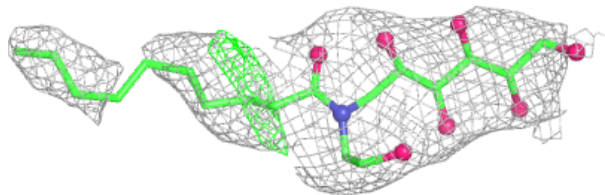
**Electron density around 2CV B 401:**

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



Electron density around 2CV A 403:

$2mF_o-DF_c$ (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.