

wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2023 – 08:20 am GMT

PDB ID : 2Y03

Title : TURKEY BETA1 ADRENERGIC RECEPTOR WITH STABILISING MU-

TATIONS AND BOUND AGONIST ISOPRENALINE

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Deposited on : 2010-11-30

Resolution : 2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

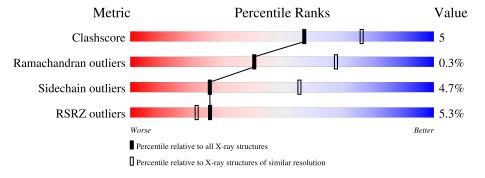
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	Similar resolution
	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 <=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	315	80%	11%	• 9%
1	В	315	82%	12%	• 5%



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4862 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called BETA-1 ADRENERGIC RECEPTOR.

\mathbf{Mol}	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
1	A	288	Total 2288	C 1510	N 377	O 381	S 20	0	0	0
1	В	298	Total 2371	C 1560	N 396	O 395	S 20	0	0	0

There are 86 discrepancies between the modelled and reference sequences:

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

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

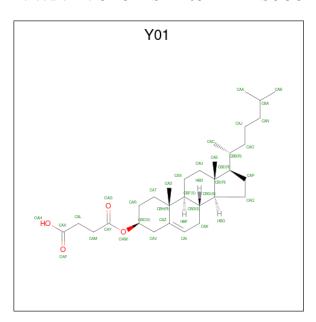
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Chain	Residue	Modelled	Actual	Comment	Reference
В	?	-	GLN	deletion	UNP P07700
В	?	-	HIS	deletion	UNP P07700
В	?	-	GLN	deletion	UNP P07700
В	?	-	PRO	deletion	UNP P07700
В	?	-	ILE	deletion	UNP P07700
В	?	-	LEU	deletion	UNP P07700
В	?	-	GLY	deletion	UNP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

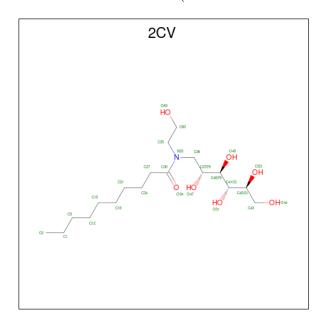
 $\bullet \ \ {\rm Molecule} \ 2 \ {\rm is} \ CHOLESTEROL \ HEMISUCCINATE \ (three-letter \ code: \ Y01) \ (formula: \ C_{31}H_{50}O_4).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
2	Λ	1	Total C O	0	0	
2	Λ	1	35 31 4		0	
2	D	1	Total C O	0	0	
	Б	1	35 31 4		0	



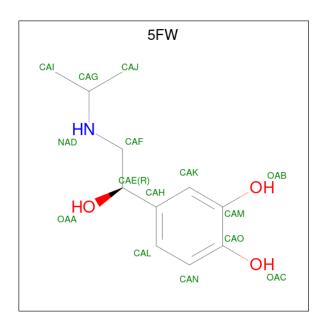
 \bullet Molecule 3 is HEGA-10 (three-letter code: 2CV) (formula: $\mathrm{C_{18}H_{37}NO_{7}}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 26 18 1 7	0	0
3	A	1	Total C 5 5	0	0
3	A	1	Total C N O 20 15 1 4	0	0
3	В	1	Total C N O 20 15 1 4	0	0
3	В	1	Total C 5 5	0	0
3	В	1	Total C N O 16 13 1 2	0	0

 \bullet Molecule 4 is ISOPRENALINE (three-letter code: 5FW) (formula: $\mathrm{C}_{11}\mathrm{H}_{17}\mathrm{NO}_3).$





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
1	Λ	1	Total	С	N	О	0	0	
4	Α	1	15	11	1	3	U	0	
1	D	1	Total	С	N	О	0	0	
4	Б	1	15	11	1	3	U	U	

• Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

• Molecule 6 is water.

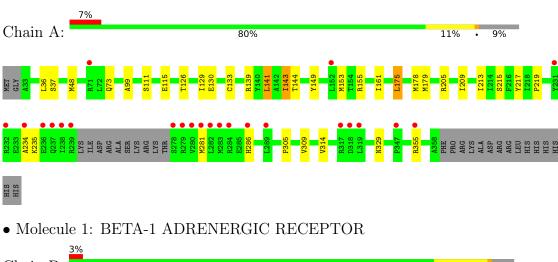
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	6	Total O 6 6	0	0
6	В	4	Total O 4 4	0	0

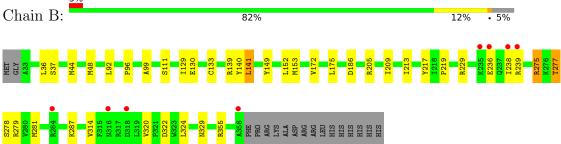


3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: BETA-1 ADRENERGIC RECEPTOR







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	89.70Å 61.60Å 101.60Å	Depositor
a, b, c, α , β , γ	90.00° 109.70° 90.00°	Depositor
Resolution (Å)	95.69 - 2.85	Depositor
rtesolution (A)	42.22 - 2.85	EDS
% Data completeness	97.0 (95.69-2.85)	Depositor
(in resolution range)	97.0 (42.22-2.85)	EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.90 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
D.D.	0.220 , 0.254	Depositor
R, R_{free}	0.225 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 58.5	EDS
L-test for twinning ²	$ < L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4862	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: Y01, 2CV, NA, 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	Bo	nd lengths	Bond angles		
Mol Chain		RMSZ	RMSZ $\# Z > 5$		# Z >5	
1	A	0.59	$1/2342 \ (0.0\%)$	0.66	0/3192	
1	В	0.60	1/2426 (0.0%)	0.68	0/3303	
All	All	0.60	$2/4768 \ (0.0\%)$	0.67	0/6495	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
1	В	133	CYS	CB-SG	-5.41	1.73	1.81
1	A	133	CYS	CB-SG	-5.02	1.73	1.81

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	on-H H(model) H(added) Clashes		Symm-Clashes	
1	A	2288	0	2373	25	0
1	В	2371	0	2471	19	0
2	A	35	0	49	2	0
2	В	35	0	49	4	0
3	A	51	0	72	5	0
3	В	41	0	59	2	0
4	A	15	0	15	0	0

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Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	$H(model) \mid H(added) \mid Clashe$		Symm-Clashes
4	В	15	0	16	0	0
5	A	1	0	0	0	0
6	A	6	0	0	0	0
6	В	4	0	0	0	0
All	All	4862	0	5104	49	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 49 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:B:205:ARG:HH12	3:B:503:2CV:H602	1.31	0.93
1:B:48:MET:HG2	1:B:99:ALA:HB1	1.64	0.78
1:A:209:ILE:HD11	1:A:314:VAL:HG11	1.68	0.75
1:A:48:MET:HG2	1:A:99:ALA:HB1	1.68	0.74
1:A:205:ARG:NH1	3:A:503:2CV:O34	2.20	0.74

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	Perce	entiles	
1	A	284/315 (90%)	276 (97%)	8 (3%)	0	100	100
1	В	296/315 (94%)	285 (96%)	9 (3%)	2 (1%)	22	50
All	All	580/630 (92%)	561 (97%)	17 (3%)	2 (0%)	41	68

All (2) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	В	186	ASP
1	В	277	THR

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	Analysed Rotameric Outliers		Percentiles		
1	A	249/273 (91%)	240 (96%)	9 (4%)	35 66		
1	В	258/273 (94%)	243 (94%)	15 (6%)	20 46		
All	All	507/546 (93%)	483 (95%)	24 (5%)	26 56		

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	175	LEU
1	В	277	THR
1	В	275	ARG
1	В	278	SER
1	A	281	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	HIS
1	В	286	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 1 is 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).

Mal	Trino	Type Chain Res I		Tiple	Во	ond leng	ths	Bond angles		
Mol	Type	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	2CV	В	503	-	15,15,25	0.90	1 (6%)	15,16,30	0.43	0
3	2CV	В	502	-	4,4,25	0.44	0	3,3,30	0.34	0
3	2CV	A	502	-	4,4,25	0.65	0	3,3,30	0.30	0
3	2CV	В	501	-	19,19,25	0.60	0	20,21,30	0.64	0
3	2CV	A	503	-	19,19,25	0.82	0	20,21,30	1.00	1 (5%)
3	2CV	A	501	-	25,25,25	0.52	0	29,30,30	1.12	3 (10%)
4	5FW	A	601	-	15,15,15	0.55	0	19,20,20	0.66	0
2	Y01	A	401	-	38,38,38	1.35	5 (13%)	57,57,57	2.22	13 (22%)
4	5FW	В	601	-	15,15,15	0.72	0	19,20,20	0.72	0
2	Y01	В	401	-	38,38,38	1.21	3 (7%)	57,57,57	1.97	13 (22%)

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
3	2CV	В	503	-	-	2/16/16/34	-
3	2CV	В	502	-	-	1/2/2/34	-
3	2CV	A	502	-	-	2/2/2/34	-
3	2CV	В	501	-	-	6/22/22/34	-
3	2CV	A	503	-	-	10/22/22/34	-
3	2CV	A	501	-	-	5/34/34/34	-
4	5FW	A	601	-	-	0/9/9/9	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Y01	A	401	-	-	11/19/77/77	0/4/4/4
4	5FW	В	601	-	-	1/9/9/9	0/1/1/1
2	Y01	В	401	-	-	10/19/77/77	0/4/4/4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	A	401	Y01	CAK-CAI	-4.56	1.40	1.50
2	В	401	Y01	CAK-CAI	-4.31	1.40	1.50
2	A	401	Y01	CAI-CAZ	3.45	1.40	1.33
2	В	401	Y01	CAI-CAZ	3.34	1.40	1.33
3	В	503	2CV	C27-C30	2.34	1.56	1.51

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	401	Y01	OAW-CBC-CAV	9.50	127.56	108.12
2	В	401	Y01	CBC-CAV-CAZ	-6.84	100.89	111.52
2	В	401	Y01	OAW-CBC-CAV	6.13	120.66	108.12
2	A	401	Y01	CAR-CBC-CAV	-4.85	103.76	110.99
2	A	401	Y01	CAC-CBB-CBE	-4.60	105.88	112.92

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	Y01	CAV-CBC-OAW-CAY
3	A	501	2CV	C41-C42-C43-O44
3	A	501	2CV	O53-C42-C43-O44
2	A	401	Y01	CAC-CBB-CBE-CAP
2	A	401	Y01	CAO-CBB-CBE-CBI

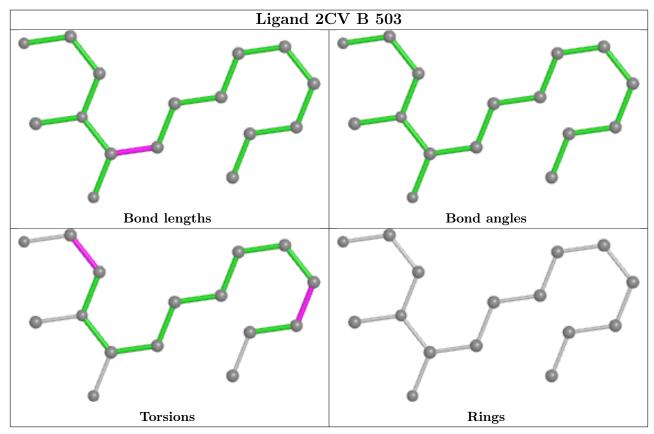
There are no ring outliers.

5 monomers are involved in 12 short contacts:

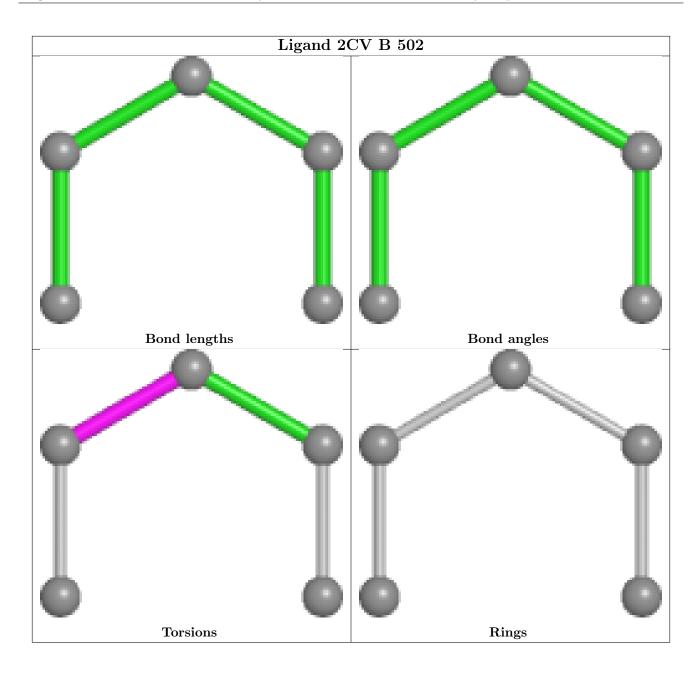
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	503	2CV	2	0
3	A	503	2CV	4	0
3	A	501	2CV	1	0
2	A	401	Y01	2	0
2	В	401	Y01	4	0



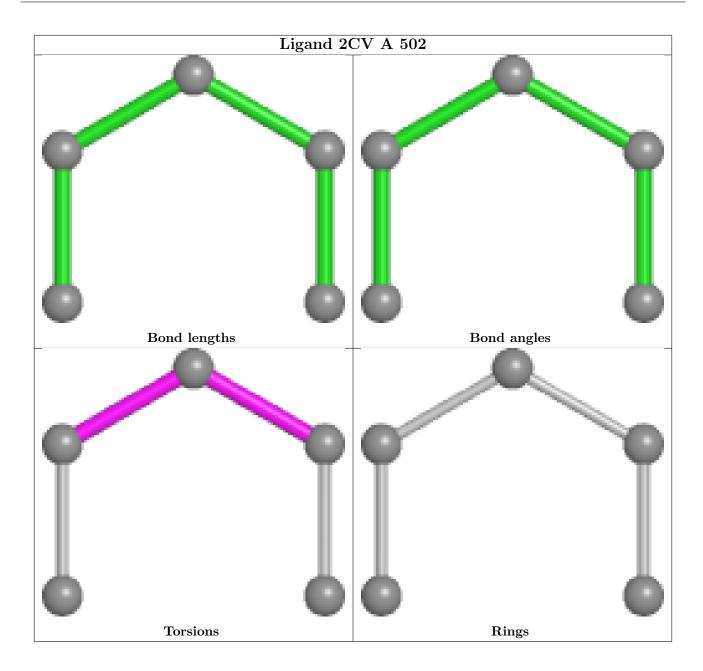
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



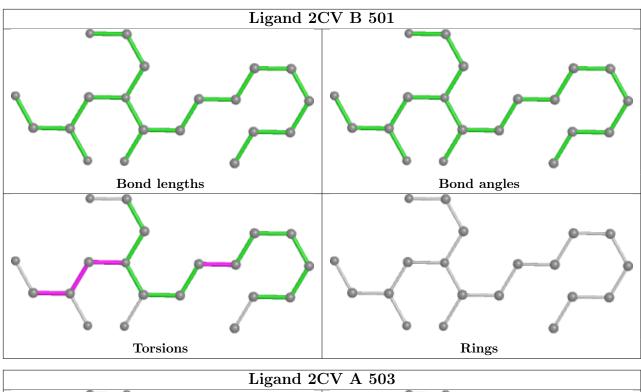


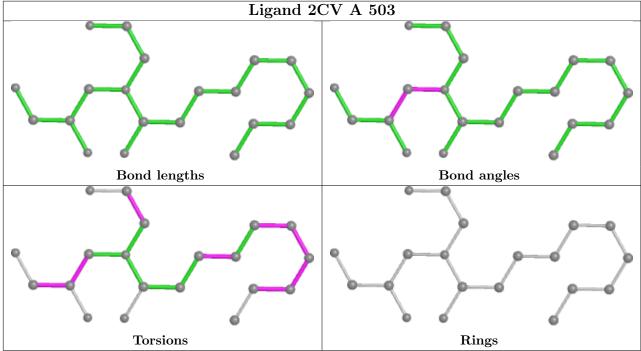




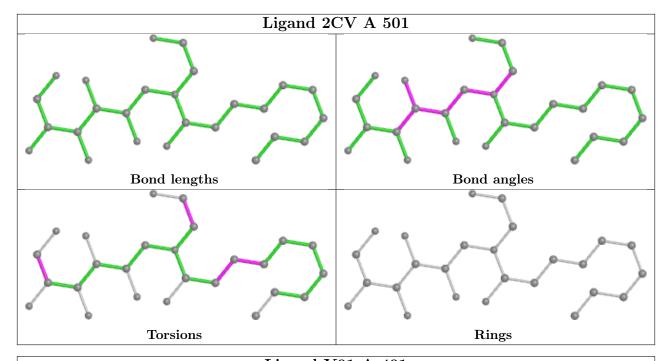


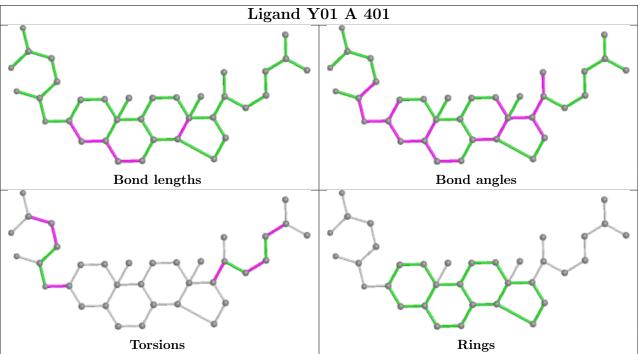




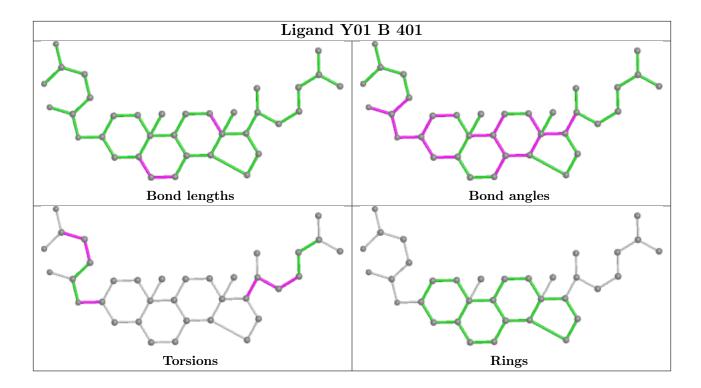












5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95^{th} 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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	288/315~(91%)	0.07	23 (7%) 12 9	28, 49, 91, 122	0
1	В	298/315~(94%)	-0.04	8 (2%) 54 50	27, 48, 80, 100	0
All	All	586/630 (93%)	0.02	31 (5%) 26 22	27, 48, 85, 122	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	ILE	5.4
1	A	281	MET	5.2
1	A	234	ALA	4.7
1	A	279	ARG	4.4
1	A	239	ARG	4.4

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 monosaccharides in this entry.

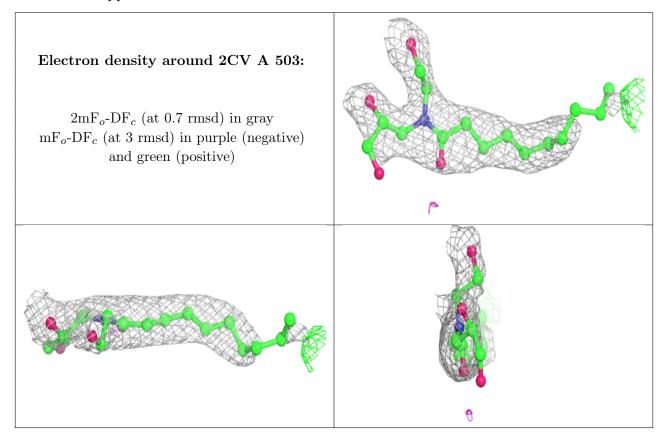
6.4 Ligands (i)

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, 95^{th} 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.

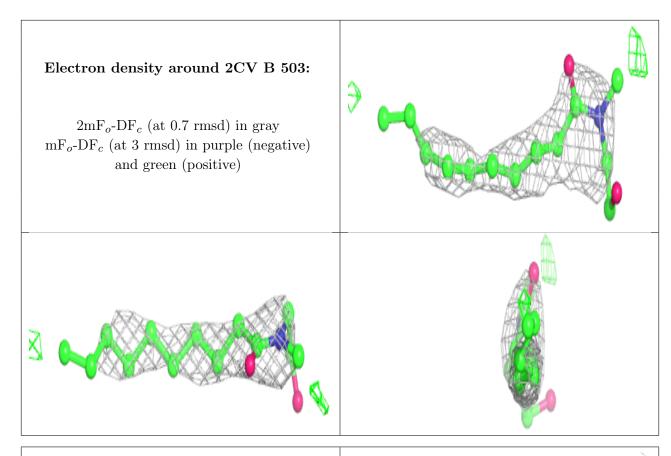


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	NA	A	701	1/1	0.51	0.18	58,58,58,58	0
3	2CV	A	503	20/26	0.81	0.34	61,85,96,96	0
3	2CV	В	503	16/26	0.85	0.60	79,87,101,104	0
3	2CV	A	501	26/26	0.85	0.25	36,66,97,100	0
3	2CV	A	502	5/26	0.88	0.31	43,51,52,54	0
3	2CV	В	501	20/26	0.89	0.29	33,63,75,79	0
2	Y01	A	401	35/35	0.94	0.22	36,45,69,72	0
4	5FW	A	601	15/15	0.96	0.19	34,37,44,45	0
2	Y01	В	401	35/35	0.96	0.21	28,35,62,68	0
4	5FW	В	601	15/15	0.97	0.21	29,38,44,45	0
3	2CV	В	502	5/26	0.98	0.17	33,42,46,46	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.

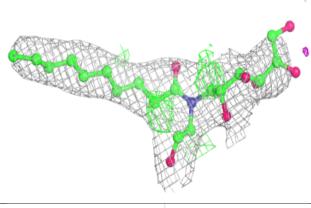


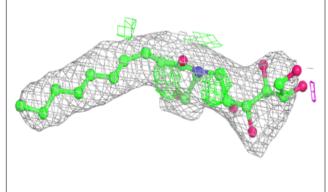


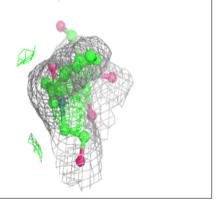


Electron density around 2CV A 501:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



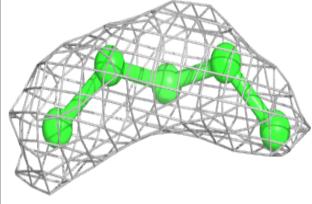


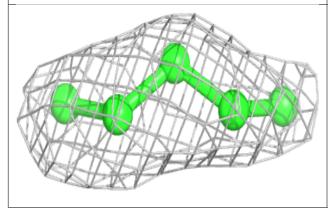


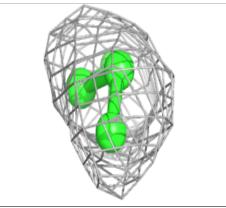


Electron density around 2CV A 502:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

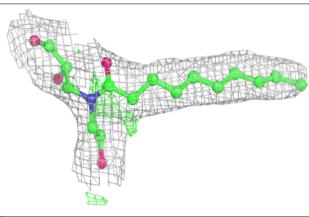


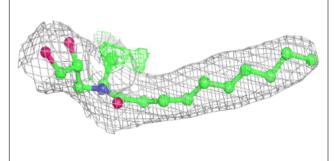


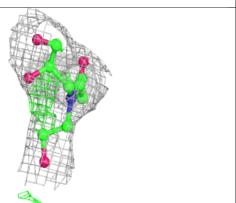


Electron density around 2CV B 501:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



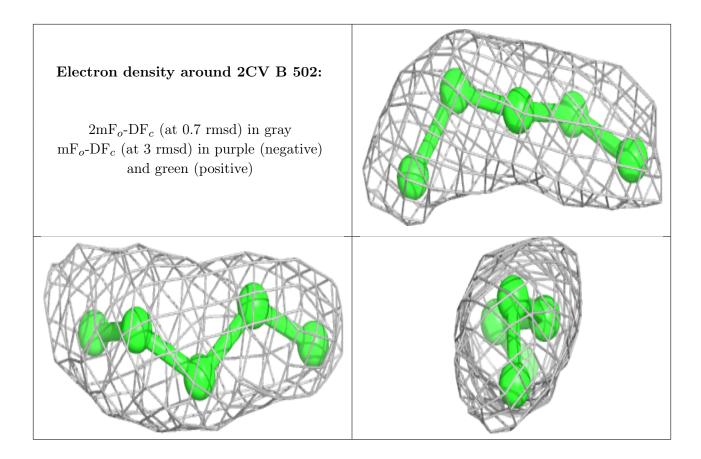






Electron density around Y01 A 401: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around Y01 B 401: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray mF_o -DF_c (at 3 rmsd) in purple (negative) and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.

