WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 07:59 pm GMT

PDB ID : 2Y00

Title : TURKEY BETA1 ADRENERGIC RECEPTOR WITH STABILISING MU-
TATIONS AND BOUND PARTIAL AGONIST DOBUTAMINE (CRYSTAL
DOB92)

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Deposited on : 2010-11-30

Resolution : 2.50 Å(reported)

The following versions of software and data (see references ①) were used in the production of this report:

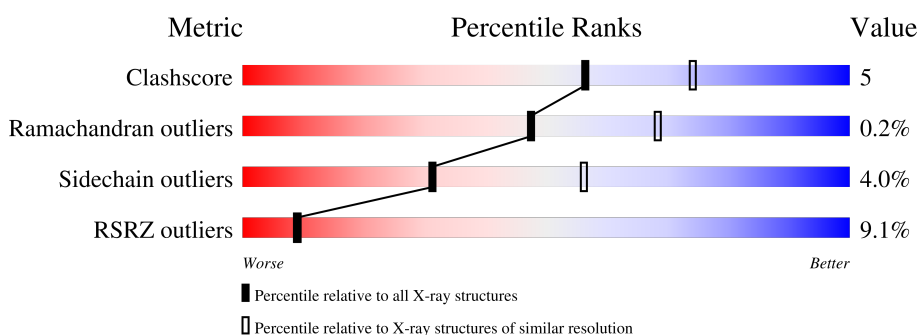|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		4.0%
RSRZ outliers		9.1%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	8% 80% 10% · 9%
1	B	315	9% 81% 12% · 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2CV	A	505	-	-	-	X
3	2CV	B	503	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2CV	B	505	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 5052 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total 2269	C 1498	N 372	O 379	S 20	0	0	0
1	B	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	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
B	31	MET	-	expression tag	UNP P07700
B	32	GLY	-	expression tag	UNP P07700
B	68	SER	ARG	engineered mutation	UNP P07700
B	90	VAL	MET	engineered mutation	UNP P07700
B	116	LEU	CYS	engineered mutation	UNP P07700
B	227	ALA	TYR	engineered mutation	UNP P07700
B	?	-	CYS	deletion	UNP P07700
B	?	-	GLU	deletion	UNP P07700
B	?	-	GLY	deletion	UNP P07700
B	?	-	ARG	deletion	UNP P07700
B	?	-	PHE	deletion	UNP P07700
B	?	-	TYR	deletion	UNP P07700
B	?	-	GLY	deletion	UNP P07700
B	?	-	SER	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	GLU	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	GLN	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700
B	?	-	LEU	deletion	UNP P07700
B	?	-	PRO	deletion	UNP P07700

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

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	31	4		
2	A	1	Total	C	O	0	0
			35	31	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total C O 35 31 4			0	0
2	B	1	Total C O 35 31 4			0	0

• Molecule 3 is HEGA-10 (three-letter code: 2CV) (formula: $C_{18}H_{37}NO_7$).
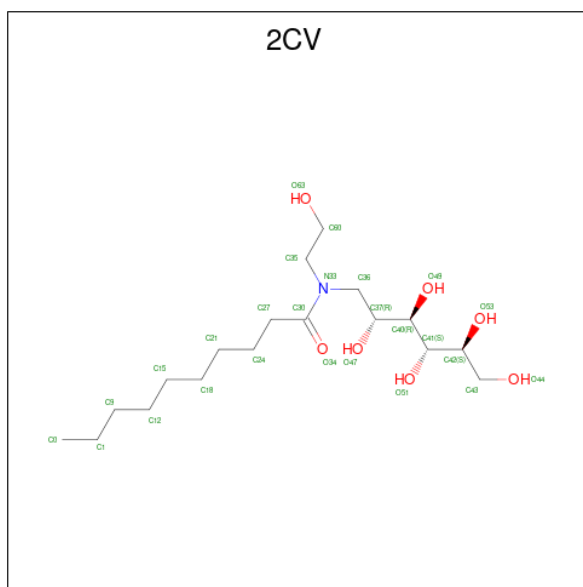
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total C N O 26 18 1 7				0	0
3	A	1	Total C 5 5				0	0
3	A	1	Total C N O 20 15 1 4				0	0
3	A	1	Total C N O 26 18 1 7				0	0
3	A	1	Total C N O 26 18 1 7				0	0
3	B	1	Total C N O 20 15 1 4				0	0
3	B	1	Total C N O 16 13 1 2				0	0
3	B	1	Total C N O 16 13 1 2				0	0
3	B	1	Total C N O 8 6 1 1				0	0

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

- Molecule 4 is DOBUTAMINE (three-letter code: Y00) (formula: $C_{18}H_{23}NO_3$).
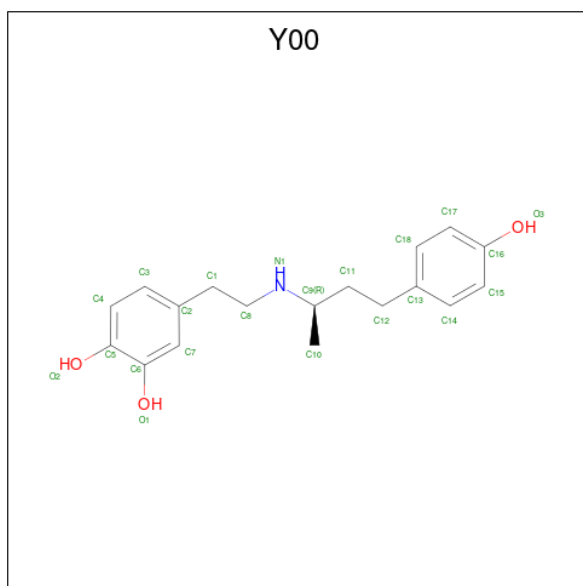
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 22	C 18	N 1	O 3	0	0
4	B	1	Total 22	C 18	N 1	O 3	0	0

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total 19	O 19	0	0
6	B	19	Total 19	O 19	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: BETA-1 ADRENERGIC RECEPTOR

Chain A:

• Molecule 1: BETA-1 ADRENERGIC RECEPTOR

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.00Å 60.50Å 101.90Å 90.00° 110.20° 90.00°	Depositor
Resolution (Å)	95.65 – 2.50 44.76 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.7 (95.65-2.50) 93.6 (44.76-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.94 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.226 , 0.256 0.228 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 75.8	EDS
L-test for twinning[2]	$<\vert L \vert> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5052	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<\vert L \vert>$, $<L^2>$ 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: NA, Y01, Y00, 2CV

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.60	1/2323 (0.0%)	0.63	0/3167
1	B	0.61	1/2426 (0.0%)	0.62	1/3303 (0.0%)
All	All	0.60	2/4749 (0.0%)	0.63	1/6470 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	CYS	CB-SG	-5.29	1.73	1.81
1	B	133	CYS	CB-SG	-5.07	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	121	ASP	CB-CG-OD1	5.05	122.84	118.30

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	2269	0	2349	20	0
1	B	2371	0	2471	24	0
2	A	70	0	98	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	70	0	98	2	0
3	A	103	0	146	5	0
3	B	86	0	122	6	0
4	A	22	0	22	3	0
4	B	22	0	20	1	0
5	A	1	0	0	0	0
6	A	19	0	0	1	0
6	B	19	0	0	2	0
All	All	5052	0	5326	52	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.

All (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:CYS:SG	3:B:505:2CV:H601	2.17	0.85
1:B:175:LEU:HB2	6:B:2010:HOH:O	1.77	0.81
3:B:501:2CV:H601	3:B:501:2CV:H272	1.68	0.75
1:A:174:PHE:O	1:A:178:MET:HG2	1.90	0.72
1:A:87:ASP:OD1	6:A:2003:HOH:O	2.07	0.72
2:A:402:Y01:HAC1	2:A:402:Y01:HAE2	1.70	0.71
1:B:235:LYS:O	1:B:238:ILE:HG13	1.94	0.68
1:B:239:ARG:O	1:B:240:LYS:HB2	1.94	0.67
3:A:505:2CV:H602	3:A:505:2CV:H37	1.77	0.66
1:B:209:ILE:HD11	1:B:314:VAL:HG11	1.78	0.65
1:A:209:ILE:HD11	1:A:314:VAL:HG11	1.82	0.62
1:B:329:ASN:OD1	4:B:601:Y00:H122	2.00	0.61
1:B:241:ILE:HD12	1:B:282:LEU:HD23	1.84	0.59
1:A:129:ILE:HG13	1:A:219:PRO:HB2	1.84	0.59
3:B:501:2CV:H272	3:B:501:2CV:C60	2.33	0.58
1:A:205:ARG:NH1	1:A:314:VAL:O	2.38	0.57
1:A:163:CYS:SG	3:A:505:2CV:H601	2.45	0.56
1:B:186:ASP:OD1	1:B:187:PRO:HD2	2.06	0.56
1:B:129:ILE:HG13	1:B:219:PRO:HB2	1.88	0.55
1:B:48:MET:HE2	1:B:330:TRP:CH2	2.44	0.52
1:B:118:THR:HG21	1:B:201:PHE:CE1	2.44	0.51
1:A:161:ILE:HG12	2:A:401:Y01:HBC	1.94	0.50
1:B:304:LEU:N	1:B:305:PRO:CD	2.75	0.49
1:B:145:SER:N	1:B:146:PRO:HD3	2.28	0.49
1:A:330:TRP:NE1	4:A:601:Y00:H17	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ILE:HD11	1:B:279:ARG:HG3	1.95	0.48
1:A:329:ASN:OD1	4:A:601:Y00:H121	2.13	0.48
1:A:205:ARG:HG2	1:A:314:VAL:HG13	1.97	0.46
1:B:69:THR:HB	1:B:72:LEU:HD12	1.98	0.46
3:A:501:2CV:H272	3:A:501:2CV:C60	2.46	0.45
1:B:130:GLU:HG2	2:B:401:Y01:HAC3	1.99	0.45
2:B:402:Y01:HAA1	3:B:505:2CV:H01C	1.99	0.44
1:A:320:VAL:HA	1:A:321:PRO:HD3	1.89	0.44
1:B:48:MET:HE2	1:B:330:TRP:HH2	1.82	0.44
1:A:118:THR:HG21	1:A:201:PHE:CE1	2.53	0.43
3:A:505:2CV:H271	3:A:505:2CV:H352	1.74	0.43
1:B:239:ARG:O	1:B:240:LYS:CB	2.63	0.43
1:B:70:GLN:HA	1:B:73:GLN:OE1	2.18	0.43
1:B:90:VAL:HA	1:B:94:VAL:HB	2.00	0.43
1:A:308:LEU:HD23	1:A:308:LEU:HA	1.83	0.43
1:B:175:LEU:N	6:B:2010:HOH:O	2.39	0.42
1:A:225:PHE:O	1:A:229:ARG:HG2	2.20	0.42
1:A:211:SER:O	1:A:215:SER:HB2	2.20	0.42
1:A:75:LEU:HD13	1:A:153:MET:HB3	2.02	0.42
1:A:182:TRP:O	1:A:203:THR:HA	2.19	0.41
1:A:317:ARG:H	1:A:317:ARG:HE	1.68	0.41
3:B:505:2CV:O47	3:B:505:2CV:H602	2.21	0.41
1:B:48:MET:HB3	1:B:48:MET:HE3	1.98	0.41
1:B:231:TYR:HD1	3:B:502:2CV:H182	1.86	0.41
1:B:195:ASP:HA	1:B:196:PRO:HD3	1.94	0.40
1:A:167:ALA:HB2	3:A:505:2CV:H181	2.03	0.40
1:A:330:TRP:HE1	4:A:601:Y00:H17	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	282/315 (90%)	274 (97%)	8 (3%)	0	100	100
1	B	296/315 (94%)	282 (95%)	13 (4%)	1 (0%)	41	61
All	All	578/630 (92%)	556 (96%)	21 (4%)	1 (0%)	47	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	240	LYS

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	247/273 (90%)	239 (97%)	8 (3%)	39	65
1	B	258/273 (94%)	246 (95%)	12 (5%)	26	49
All	All	505/546 (92%)	485 (96%)	20 (4%)	31	56

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	SER
1	A	53	LEU
1	A	175	LEU
1	A	188	GLN
1	A	235	LYS
1	A	278	SER
1	A	317	ARG
1	A	329	ASN
1	B	37	SER
1	B	53	LEU
1	B	70	GLN
1	B	71	ARG
1	B	111	SER
1	B	129	ILE
1	B	175	LEU

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Mol	Chain	Res	Type
1	B	235	LYS
1	B	236	GLU
1	B	275	ARG
1	B	317	ARG
1	B	329	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	#$|Z| > 2$
3	2CV	A	501	-	25,25,25	0.82	0	29,30,30	1.22	3 (10%)
2	Y01	B	402	-	38,38,38	1.32	2 (5%)	57,57,57	1.53	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	2CV	A	505	-	25,25,25	0.78	0	29,30,30	0.92	1 (3%)
3	2CV	B	502	-	15,15,25	0.86	1 (6%)	15,16,30	0.36	0
3	2CV	B	501	-	19,19,25	0.54	0	20,21,30	0.94	1 (5%)
3	2CV	A	504	-	25,25,25	0.61	0	29,30,30	1.45	2 (6%)
4	Y00	B	601	-	23,23,23	1.08	1 (4%)	29,30,30	1.42	1 (3%)
3	2CV	A	503	-	19,19,25	0.61	0	20,21,30	0.47	0
3	2CV	B	504	-	7,7,25	0.79	0	7,7,30	0.25	0
2	Y01	A	402	-	38,38,38	1.42	3 (7%)	57,57,57	1.44	8 (14%)
3	2CV	A	502	-	4,4,25	0.49	0	3,3,30	0.35	0
3	2CV	B	505	-	25,25,25	0.75	0	29,30,30	0.72	1 (3%)
2	Y01	A	401	-	38,38,38	1.28	2 (5%)	57,57,57	1.88	16 (28%)
3	2CV	B	503	-	15,15,25	0.68	0	15,16,30	0.63	0
4	Y00	A	601	-	23,23,23	1.25	1 (4%)	29,30,30	1.08	2 (6%)
2	Y01	B	401	-	38,38,38	1.24	3 (7%)	57,57,57	1.91	14 (24%)

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	A	501	-	-	14/34/34/34	-
2	Y01	B	402	-	-	11/19/77/77	0/4/4/4
3	2CV	A	505	-	-	14/34/34/34	-
3	2CV	B	502	-	-	4/16/16/34	-
3	2CV	B	501	-	-	7/22/22/34	-
3	2CV	A	504	-	-	22/34/34/34	-
4	Y00	B	601	-	-	2/11/11/11	0/2/2/2
3	2CV	A	503	-	-	9/22/22/34	-
3	2CV	B	504	-	-	0/5/5/34	-
2	Y01	A	402	-	-	12/19/77/77	0/4/4/4
3	2CV	A	502	-	-	0/2/2/34	-
3	2CV	B	505	-	-	11/34/34/34	-
2	Y01	A	401	-	-	11/19/77/77	0/4/4/4
3	2CV	B	503	-	-	1/16/16/34	-
4	Y00	A	601	-	-	5/11/11/11	0/2/2/2
2	Y01	B	401	-	-	10/19/77/77	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	Y01	CAK-CAI	-5.16	1.39	1.50
4	A	601	Y00	C5-C6	5.07	1.48	1.40
2	A	402	Y01	CAK-CAI	-4.84	1.39	1.50
2	A	401	Y01	CAK-CAI	-4.60	1.40	1.50
4	B	601	Y00	C5-C6	4.43	1.47	1.40
2	B	401	Y01	CAK-CAI	-4.29	1.41	1.50
2	A	402	Y01	CAI-CAZ	3.37	1.40	1.33
2	A	401	Y01	CAI-CAZ	3.30	1.40	1.33
2	B	401	Y01	CAI-CAZ	3.22	1.40	1.33
2	A	402	Y01	CBH-CAZ	2.53	1.57	1.52
2	B	402	Y01	CAI-CAZ	2.51	1.38	1.33
3	B	502	2CV	C27-C30	2.31	1.56	1.51
2	B	401	Y01	CAV-CAZ	2.11	1.56	1.51

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	Y01	OAW-CBC-CAV	5.58	119.54	108.12
4	B	601	Y00	C8-N1-C9	5.36	122.15	114.05
2	B	401	Y01	OAW-CBC-CAV	5.20	118.76	108.12
2	B	401	Y01	OAW-CBC-CAR	5.18	120.82	108.33
2	A	402	Y01	OAW-CAY-CAM	5.16	122.62	111.50
2	B	401	Y01	CBC-CAV-CAZ	-5.13	103.55	111.52
3	A	504	2CV	C37-C40-C41	5.08	120.42	112.47
2	B	402	Y01	CAV-CAZ-CBH	4.72	122.69	116.42
2	A	401	Y01	CAR-CBC-CAV	-4.23	104.68	110.99
2	B	402	Y01	OAW-CAY-CAM	4.01	120.15	111.50
2	A	401	Y01	CAV-CAZ-CBH	3.96	121.68	116.42
2	A	401	Y01	OAW-CBC-CAR	3.94	117.84	108.33
2	A	402	Y01	CAV-CAZ-CBH	3.92	121.63	116.42
3	A	501	2CV	C35-N33-C36	-3.75	111.94	116.41
3	A	504	2CV	C42-C41-C40	-3.65	106.75	112.47
4	A	601	Y00	C8-N1-C9	3.53	119.38	114.05
2	B	402	Y01	OAW-CBC-CAV	-3.46	101.03	108.12
2	A	401	Y01	OAW-CAY-CAM	3.43	118.89	111.50
2	B	401	Y01	CAO-CBB-CBE	3.37	117.25	110.28
2	B	401	Y01	CAR-CBC-CAV	-3.35	105.99	110.99
2	B	401	Y01	CAC-CBB-CBE	-3.34	107.81	112.92
2	A	401	Y01	CAC-CBB-CBE	-3.21	108.00	112.92
2	B	402	Y01	CAV-CAZ-CAI	-3.20	115.99	120.61
2	B	401	Y01	CAT-CAR-CBC	-3.01	105.19	110.33
2	A	402	Y01	CAK-CBD-CBF	2.89	113.21	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	505	2CV	C37-C40-C41	2.88	116.97	112.47
2	A	401	Y01	CAT-CBH-CBF	2.87	112.73	108.73
2	B	402	Y01	OAW-CBC-CAR	2.87	115.25	108.33
2	B	401	Y01	OAW-CAY-CAM	2.83	117.59	111.50
2	B	402	Y01	CAQ-CBG-CBI	-2.81	100.46	103.84
2	A	401	Y01	CAO-CBB-CBE	2.78	116.03	110.28
2	A	401	Y01	CBF-CBD-CBG	2.74	112.76	109.09
4	A	601	Y00	C11-C9-N1	2.73	114.17	110.00
2	B	401	Y01	CAP-CBE-CBB	2.73	116.37	112.15
2	B	402	Y01	CBG-CBI-CBE	-2.72	96.85	100.07
3	B	501	2CV	C35-N33-C36	-2.59	113.33	116.41
2	A	402	Y01	CAV-CAZ-CAI	-2.57	116.90	120.61
2	A	402	Y01	OAW-CAY-OAG	-2.52	117.62	123.70
2	A	401	Y01	OAF-CAX-CAL	-2.47	115.15	123.08
2	A	401	Y01	CAP-CBE-CBB	2.46	115.96	112.15
2	A	401	Y01	CBC-CAV-CAZ	-2.44	107.72	111.52
2	B	401	Y01	CAU-CBI-CBE	-2.38	113.01	116.57
2	B	401	Y01	CAV-CAZ-CBH	2.34	119.53	116.42
2	B	402	Y01	CAP-CBE-CBB	-2.31	108.58	112.15
2	B	402	Y01	OAW-CAY-OAG	-2.29	118.17	123.70
2	A	401	Y01	CBI-CBE-CBB	-2.28	115.92	119.49
2	A	402	Y01	CBG-CBI-CBE	-2.27	97.38	100.07
2	A	401	Y01	CBG-CBI-CBE	-2.22	97.44	100.07
2	B	401	Y01	CBH-CAZ-CAI	-2.19	119.56	122.90
3	B	505	2CV	C42-C41-C40	2.18	115.88	112.47
2	B	401	Y01	OAF-CAX-CAL	-2.17	116.10	123.08
2	A	401	Y01	CAU-CBI-CBE	-2.13	113.39	116.57
2	A	402	Y01	CAU-CBI-CBE	-2.12	113.40	116.57
3	A	501	2CV	O51-C41-C42	2.09	113.87	108.81
2	A	401	Y01	CAD-CBH-CBF	-2.07	109.21	111.68
2	A	402	Y01	CAD-CBH-CAZ	2.05	111.67	108.34
2	B	401	Y01	CAL-CAM-CAY	-2.05	107.47	113.43
3	A	501	2CV	C37-C40-C41	2.05	115.67	112.47
2	B	402	Y01	CAK-CBD-CBF	2.04	112.18	109.71
2	B	402	Y01	OAF-CAX-CAL	-2.00	116.64	123.08

There are no chirality outliers.

All (133) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	Y01	CAR-CBC-OAW-CAY
2	A	402	Y01	OAG-CAY-OAW-CBC

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Mol	Chain	Res	Type	Atoms
2	A	402	Y01	CAM-CAY-OAW-CBC
2	B	401	Y01	CAR-CBC-OAW-CAY
2	B	402	Y01	CAR-CBC-OAW-CAY
2	B	402	Y01	OAG-CAY-OAW-CBC
3	A	501	2CV	C37-C36-N33-C30
3	A	501	2CV	C37-C36-N33-C35
3	A	501	2CV	N33-C36-C37-O47
3	A	501	2CV	C36-C37-C40-C41
3	A	501	2CV	C36-C37-C40-O49
3	A	501	2CV	O47-C37-C40-C41
3	A	501	2CV	O47-C37-C40-O49
3	A	501	2CV	C37-C40-C41-C42
3	A	501	2CV	C37-C40-C41-O51
3	A	501	2CV	O49-C40-C41-C42
3	A	501	2CV	O49-C40-C41-O51
3	A	503	2CV	C36-C37-C40-O49
3	A	504	2CV	N33-C36-C37-C40
3	A	504	2CV	N33-C36-C37-O47
3	A	504	2CV	C36-C37-C40-C41
3	A	504	2CV	C36-C37-C40-O49
3	A	504	2CV	O47-C37-C40-C41
3	A	504	2CV	O47-C37-C40-O49
3	A	504	2CV	C37-C40-C41-C42
3	A	504	2CV	C37-C40-C41-O51
3	A	504	2CV	O49-C40-C41-C42
3	A	504	2CV	O49-C40-C41-O51
3	A	504	2CV	O51-C41-C42-C43
3	A	505	2CV	N33-C35-C60-O63
3	A	505	2CV	N33-C36-C37-C40
3	A	505	2CV	N33-C36-C37-O47
3	A	505	2CV	C36-C37-C40-C41
3	A	505	2CV	C36-C37-C40-O49
3	B	501	2CV	N33-C36-C37-C40
3	B	501	2CV	N33-C36-C37-O47
3	B	505	2CV	N33-C35-C60-O63
3	B	505	2CV	C37-C40-C41-C42
3	B	505	2CV	C37-C40-C41-O51
3	B	505	2CV	O53-C42-C43-O44
4	A	601	Y00	C12-C11-C9-C10
4	A	601	Y00	C12-C11-C9-N1
2	A	402	Y01	CAC-CBB-CBE-CBI
3	B	502	2CV	C21-C24-C27-C30

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Mol	Chain	Res	Type	Atoms
2	B	402	Y01	CAM-CAY-OAW-CBC
2	A	401	Y01	CAC-CBB-CBE-CAP
3	A	504	2CV	C21-C24-C27-C30
3	A	504	2CV	N33-C35-C60-O63
3	B	505	2CV	C41-C42-C43-O44
2	A	402	Y01	CAO-CBB-CBE-CAP
3	A	504	2CV	O51-C41-C42-O53
3	A	504	2CV	C40-C41-C42-O53
3	B	505	2CV	O49-C40-C41-O51
3	A	504	2CV	C40-C41-C42-C43
2	A	401	Y01	CAC-CBB-CBE-CBI
2	A	401	Y01	CAO-CBB-CBE-CBI
2	B	401	Y01	CAO-CBB-CBE-CBI
2	B	401	Y01	CAX-CAL-CAM-CAY
2	A	402	Y01	CAC-CBB-CBE-CAP
2	B	401	Y01	CAC-CBB-CBE-CAP
2	A	401	Y01	CAO-CBB-CBE-CAP
2	B	401	Y01	CAN-CAJ-CAO-CBB
2	A	401	Y01	CAN-CAJ-CAO-CBB
3	A	503	2CV	O47-C37-C40-O49
3	B	505	2CV	O49-C40-C41-C42
3	A	504	2CV	C41-C42-C43-O44
2	B	401	Y01	CAC-CBB-CBE-CBI
2	A	401	Y01	CAX-CAL-CAM-CAY
3	A	504	2CV	O53-C42-C43-O44
3	A	505	2CV	O47-C37-C40-O49
3	A	504	2CV	C18-C21-C24-C27
2	A	402	Y01	CAX-CAL-CAM-CAY
3	A	504	2CV	C9-C12-C15-C18
3	B	501	2CV	N33-C35-C60-O63
3	B	502	2CV	C9-C12-C15-C18
3	B	505	2CV	C21-C24-C27-C30
3	A	503	2CV	C15-C12-C9-C1
2	B	402	Y01	CAJ-CAN-CBA-CAB
3	A	505	2CV	C37-C40-C41-O51
2	A	401	Y01	CAJ-CAN-CBA-CAB
2	B	401	Y01	CAO-CBB-CBE-CAP
3	A	505	2CV	C37-C40-C41-C42
2	B	401	Y01	CAJ-CAN-CBA-CAB
2	A	402	Y01	CAJ-CAO-CBB-CBE
2	A	401	Y01	CAJ-CAN-CBA-CAA
2	B	401	Y01	CAJ-CAN-CBA-CAA

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Mol	Chain	Res	Type	Atoms
3	A	505	2CV	O47-C37-C40-C41
2	B	402	Y01	CAV-CBC-OAW-CAY
3	A	501	2CV	N33-C35-C60-O63
3	B	505	2CV	C15-C12-C9-C1
3	A	504	2CV	C0-C1-C9-C12
2	B	402	Y01	CAO-CAJ-CAN-CBA
2	B	402	Y01	CAJ-CAN-CBA-CAA
2	A	402	Y01	CAO-CBB-CBE-CBI
3	A	503	2CV	C21-C24-C27-C30
3	A	503	2CV	C0-C1-C9-C12
3	A	503	2CV	C18-C21-C24-C27
3	A	504	2CV	C15-C12-C9-C1
3	B	501	2CV	C60-C35-N33-C36
3	B	501	2CV	O47-C37-C40-O49
4	B	601	Y00	C8-C1-C2-C3
4	B	601	Y00	C8-C1-C2-C7
3	B	502	2CV	N33-C35-C60-O63
3	A	503	2CV	C9-C12-C15-C18
3	A	505	2CV	C9-C12-C15-C18
3	A	505	2CV	C15-C12-C9-C1
3	A	505	2CV	C21-C24-C27-C30
3	B	501	2CV	C60-C35-N33-C30
3	A	503	2CV	N33-C36-C37-O47
2	A	402	Y01	CAJ-CAO-CBB-CAC
2	A	402	Y01	CAM-CAL-CAX-OAF
2	B	402	Y01	CAM-CAL-CAX-OAF
2	A	401	Y01	CAM-CAL-CAX-OAH
2	A	402	Y01	CAM-CAL-CAX-OAH
2	A	401	Y01	CAM-CAL-CAX-OAF
2	B	402	Y01	CAM-CAL-CAX-OAH
4	A	601	Y00	C11-C12-C13-C14
3	B	505	2CV	C9-C12-C15-C18
4	A	601	Y00	C11-C12-C13-C18
3	B	501	2CV	C36-C37-C40-O49
2	A	402	Y01	CAL-CAM-CAY-OAW
3	A	501	2CV	C21-C24-C27-C30
3	A	505	2CV	O51-C41-C42-C43
3	B	502	2CV	C0-C1-C9-C12
3	B	503	2CV	C15-C18-C21-C24
3	B	505	2CV	C15-C18-C21-C24
4	A	601	Y00	C11-C9-N1-C8
2	B	402	Y01	CAJ-CAO-CBB-CBE

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Mol	Chain	Res	Type	Atoms
3	A	505	2CV	C40-C41-C42-C43
3	A	501	2CV	N33-C36-C37-C40
2	B	402	Y01	CAL-CAM-CAY-OAW
3	A	503	2CV	N33-C36-C37-C40
2	B	401	Y01	CAL-CAM-CAY-OAW

There are no ring outliers.

11 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	2CV	1	0
2	B	402	Y01	1	0
3	A	505	2CV	4	0
3	B	502	2CV	1	0
3	B	501	2CV	2	0
4	B	601	Y00	1	0
2	A	402	Y01	1	0
3	B	505	2CV	3	0
2	A	401	Y01	1	0
4	A	601	Y00	3	0
2	B	401	Y01	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 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.

Ligand 2CV A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand Y01 B 402

Bond lengths

Bond angles

Torsions

Rings

Ligand 2CV A 505

Bond lengths

Bond angles

Torsions

Rings

Ligand 2CV B 502

Bond lengths

Bond angles

Torsions

Rings

Ligand 2CV B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 2CV A 504

Bond lengths

Bond angles

Torsions

Rings

Ligand Y00 B 601

Bond lengths

Bond angles

Torsions

Rings

Ligand 2CV A 503

Bond lengths

Bond angles

Torsions

Rings

Ligand Y01 A 402

Bond lengths

Bond angles

Torsions

Rings

Ligand 2CV B 505

Bond lengths

Bond angles

Torsions

Rings

Ligand Y01 A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand 2CV B 503

Bond lengths

Bond angles

Torsions

Rings

Ligand Y00 A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand Y01 B 401

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	286/315 (90%)	0.49	24 (8%)	11	11	10, 32, 76, 101	0
1	B	298/315 (94%)	0.58	29 (9%)	7	7	10, 30, 84, 99	0
All	All	584/630 (92%)	0.54	53 (9%)	9	9	10, 31, 79, 101	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	358	ALA	9.2
1	B	277	THR	7.8
1	B	241	ILE	7.7
1	A	279	ARG	7.6
1	B	280	VAL	6.7
1	B	242	ASP	5.9
1	B	281	MET	5.5
1	A	283	MET	5.4
1	A	318	ASP	5.3
1	A	319	LEU	5.2
1	A	235	LYS	4.9
1	B	278	SER	4.7
1	A	147	PHE	4.6
1	B	357	LEU	4.6
1	A	316	ASN	4.2
1	A	281	MET	4.2
1	A	278	SER	4.2
1	B	238	ILE	3.9
1	B	356	LEU	3.9
1	A	280	VAL	3.9
1	B	283	MET	3.8
1	B	351	LYS	3.7
1	B	239	ARG	3.5
1	A	284	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	274	LYS	3.4
1	B	276	LYS	3.4
1	A	231	TYR	3.4
1	B	236	GLU	3.3
1	B	319	LEU	3.3
1	A	234	ALA	3.2
1	A	34	GLU	3.1
1	B	349	PHE	3.0
1	B	355	ARG	3.0
1	B	235	LYS	2.9
1	B	279	ARG	2.8
1	A	323	TRP	2.8
1	A	321	PRO	2.8
1	B	70	GLN	2.8
1	B	40	TRP	2.7
1	B	284	ARG	2.6
1	A	285	GLU	2.6
1	B	318	ASP	2.6
1	A	358	ALA	2.5
1	B	348	ASP	2.5
1	A	237	GLN	2.4
1	A	320	VAL	2.4
1	A	351	LYS	2.4
1	A	354	LYS	2.4
1	A	152	LEU	2.1
1	B	282	LEU	2.1
1	B	346	SER	2.1
1	B	243	ARG	2.1
1	A	282	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	2CV	A	505	26/26	0.50	0.43	57,93,108,109	0
3	2CV	B	505	26/26	0.51	0.47	59,90,103,105	0
3	2CV	A	503	20/26	0.66	0.40	53,81,98,98	0
3	2CV	B	503	16/26	0.69	0.47	79,84,103,107	0
2	Y01	A	402	35/35	0.69	0.34	55,67,99,101	0
3	2CV	A	504	26/26	0.71	0.27	43,77,85,86	0
3	2CV	B	502	16/26	0.73	0.39	23,73,88,90	0
5	NA	A	1359	1/1	0.75	0.18	40,40,40,40	0
3	2CV	A	501	26/26	0.77	0.25	14,54,75,79	0
3	2CV	B	504	8/26	0.81	0.25	30,47,56,60	0
3	2CV	A	502	5/26	0.85	0.19	39,40,43,44	0
3	2CV	B	501	20/26	0.86	0.30	16,47,60,65	0
4	Y00	B	601	22/22	0.90	0.22	21,30,37,39	0
2	Y01	A	401	35/35	0.90	0.23	18,26,50,58	0
2	Y01	B	402	35/35	0.91	0.26	27,35,84,86	0
4	Y00	A	601	22/22	0.91	0.23	27,35,50,59	0
2	Y01	B	401	35/35	0.95	0.20	10,25,46,50	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 505:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
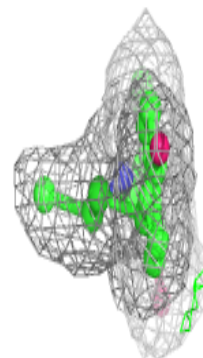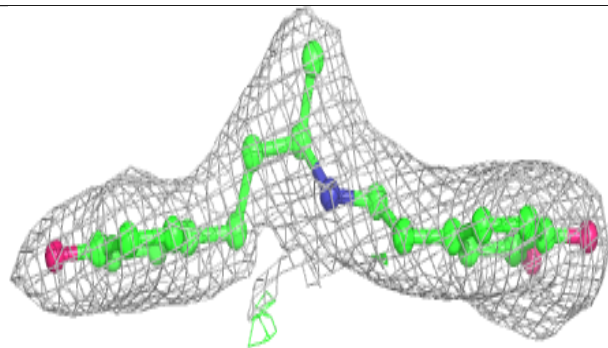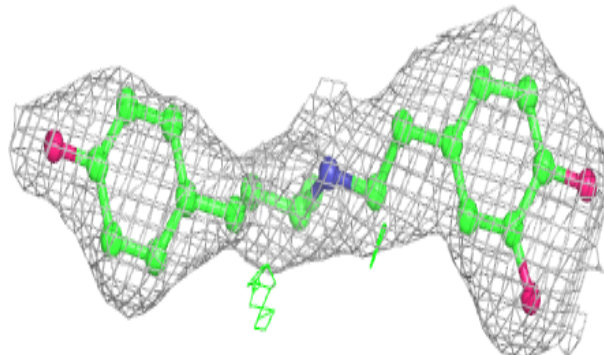$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
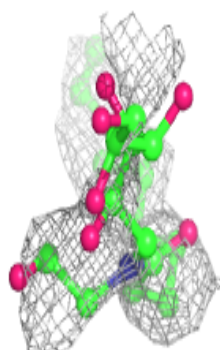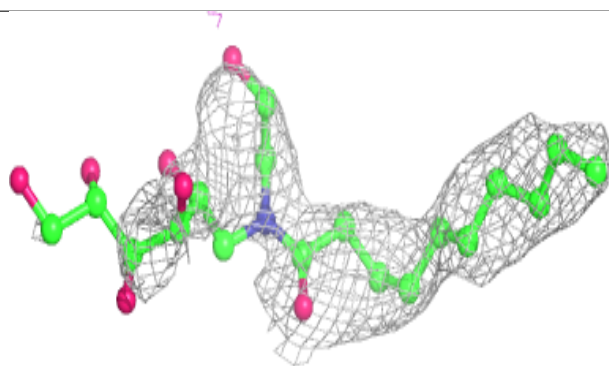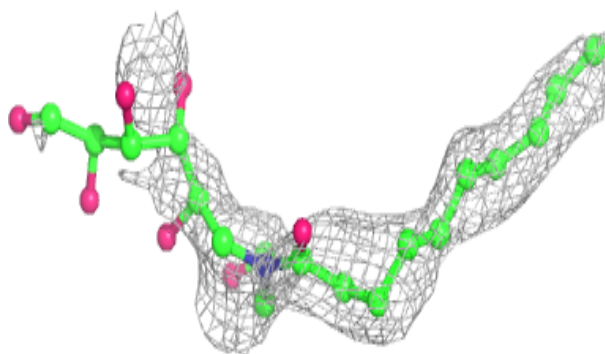
Electron density around 2CV B 505:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
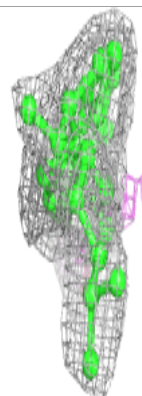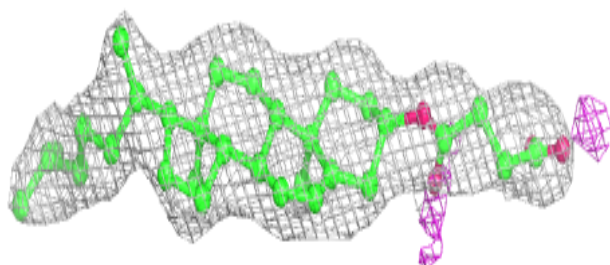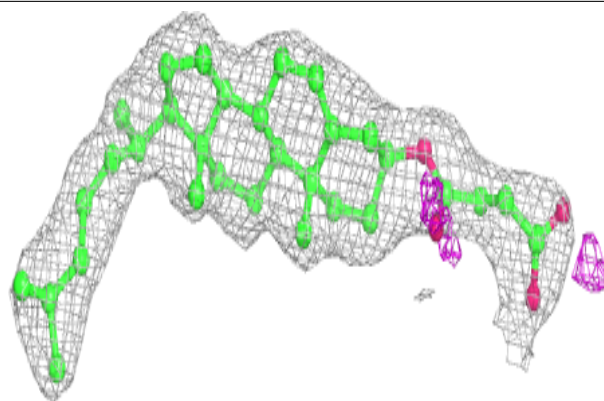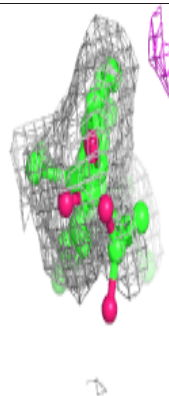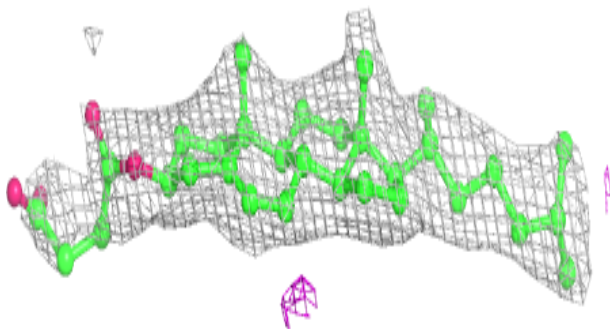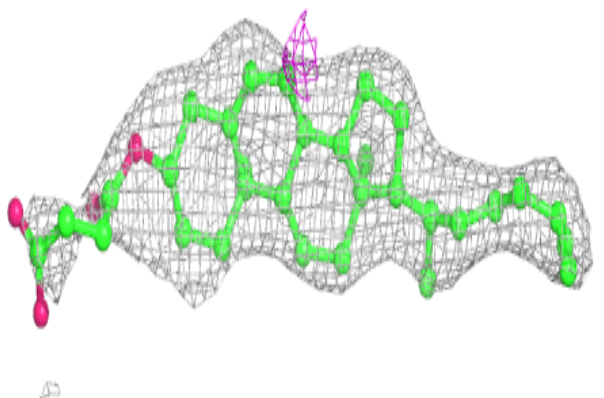and green (positive)
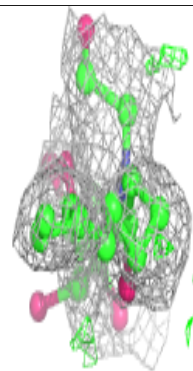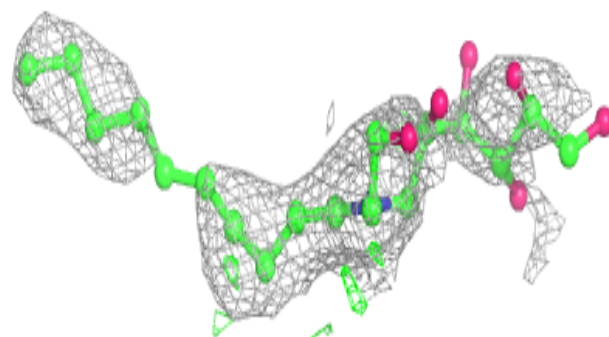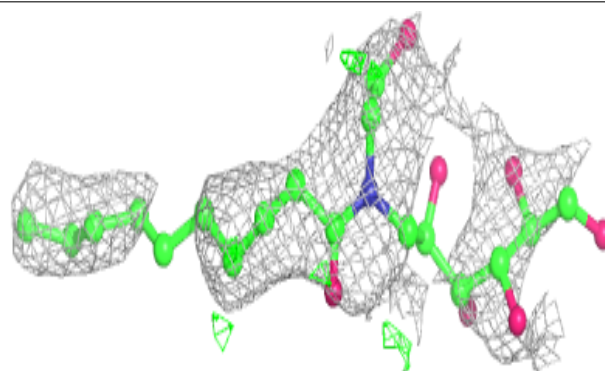
Electron density around 2CV A 503:
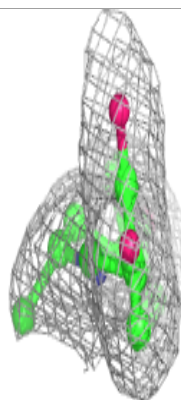
$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
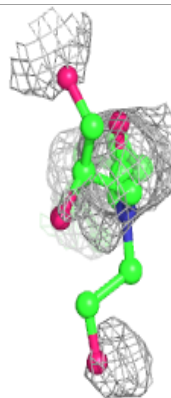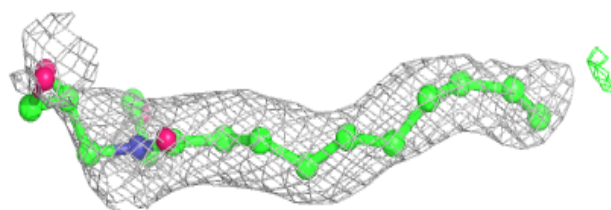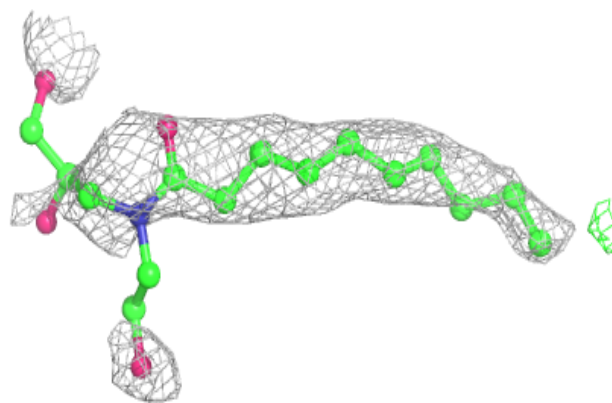
Electron density around 2CV B 503:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
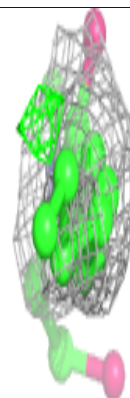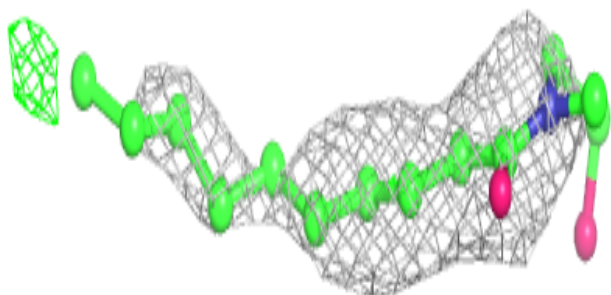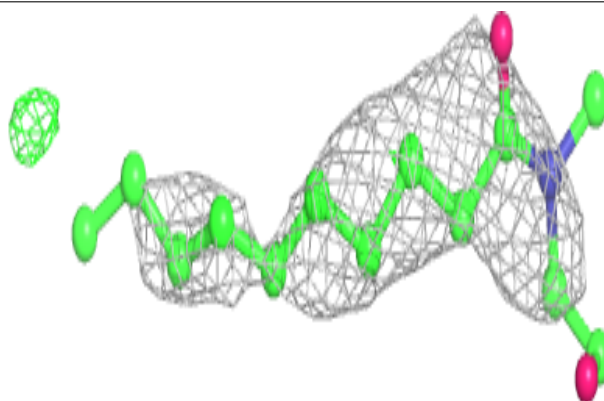
Electron density around Y01 A 402:
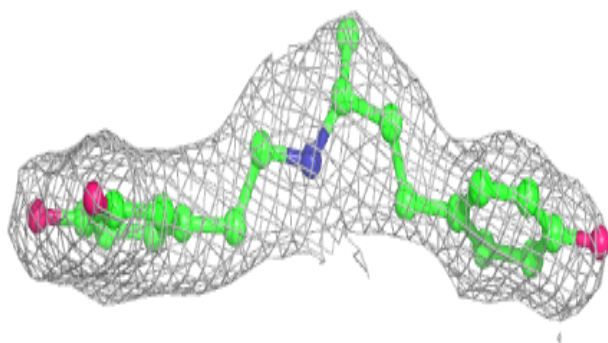
$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
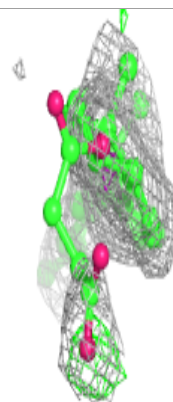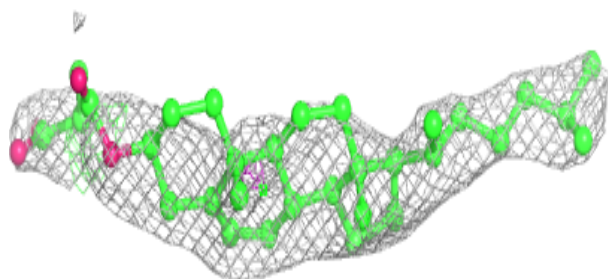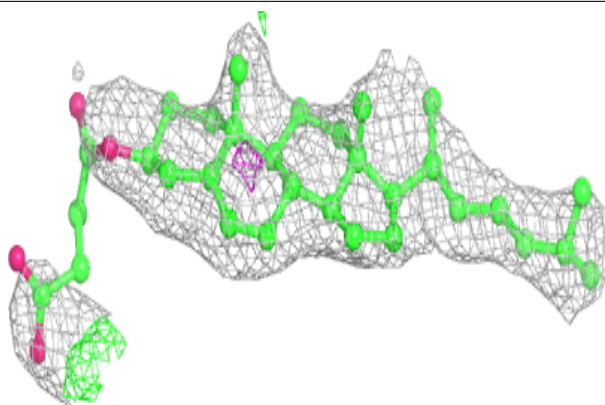
Electron density around 2CV A 504:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
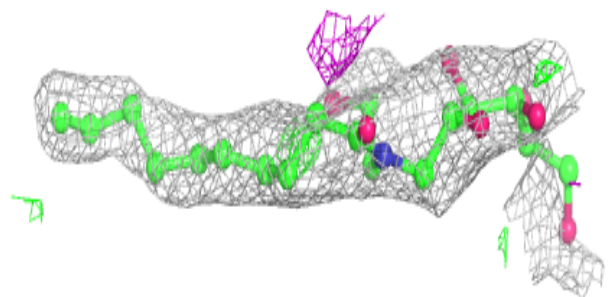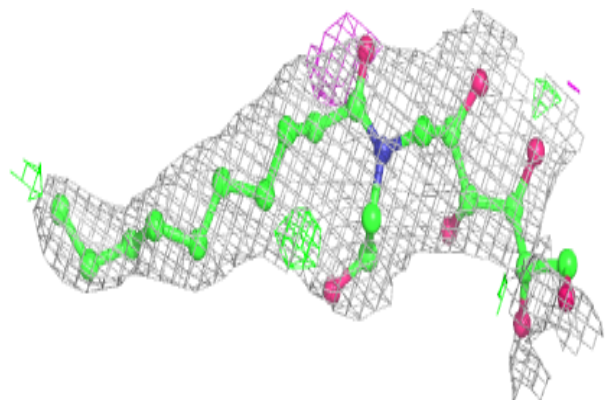
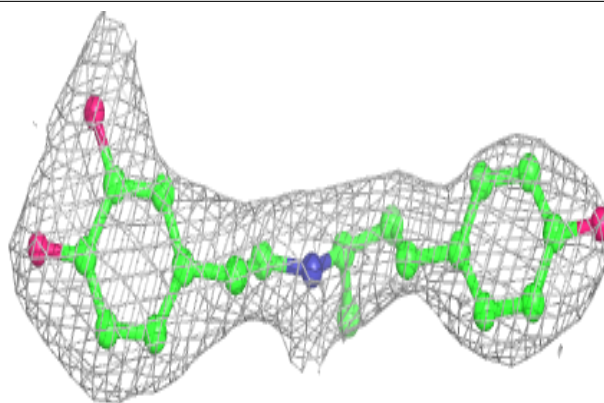**Electron density around 2CV B 502:**

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
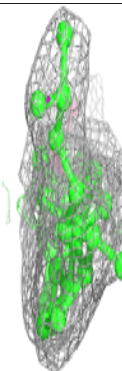and green (positive)
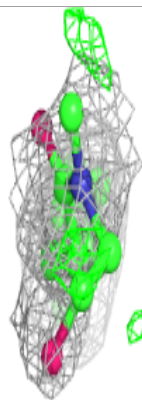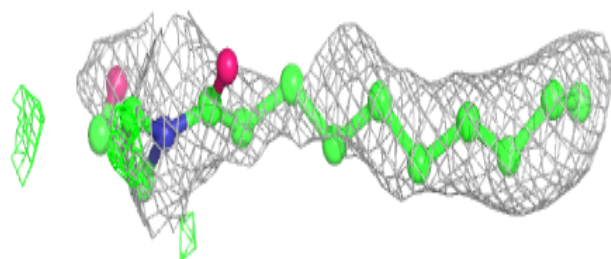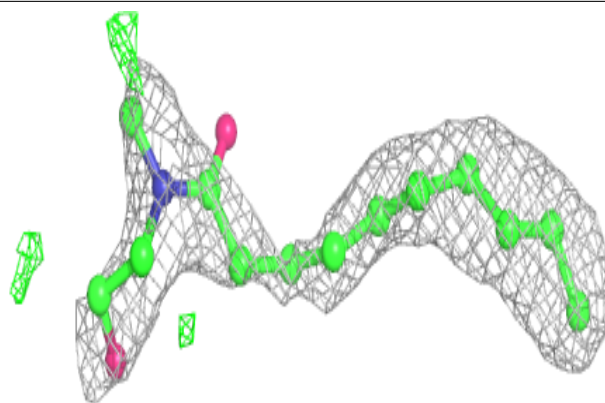
Electron density around 2CV A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
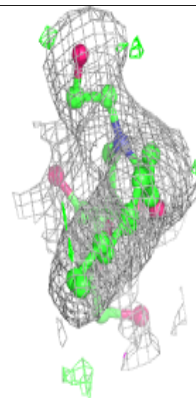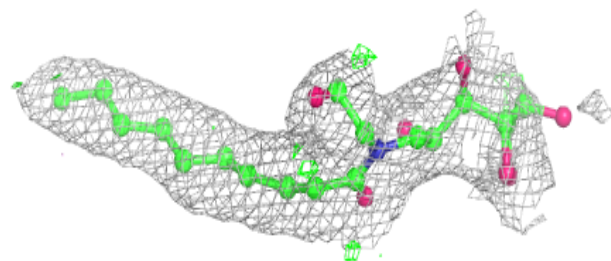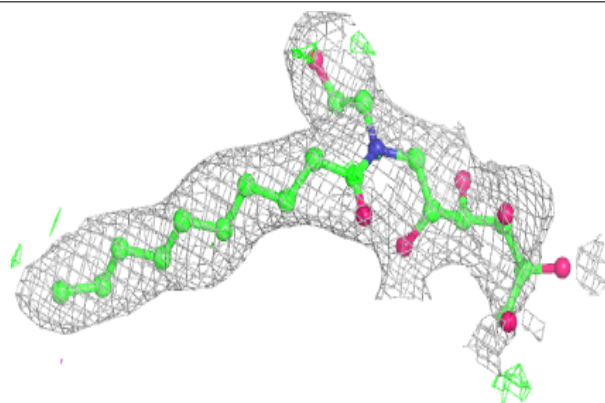
Electron density around 2CV B 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
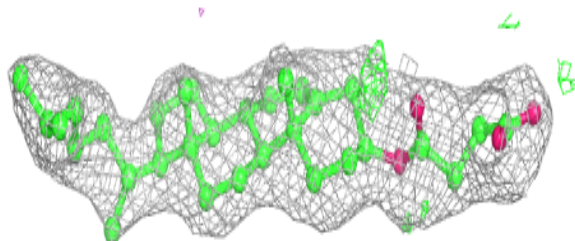and green (positive)
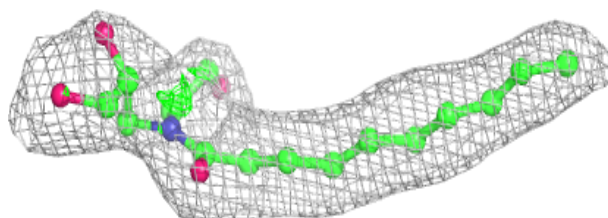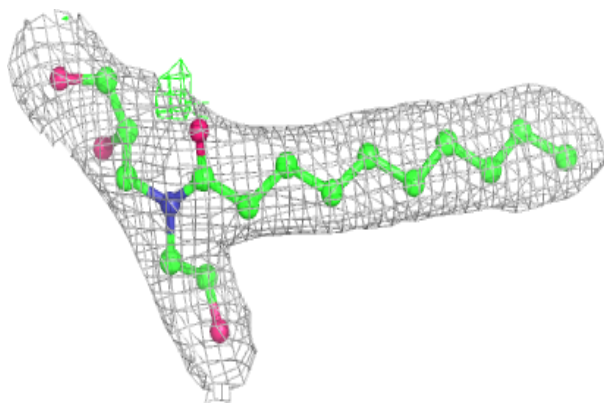
Electron density around Y00 B 601:

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

Electron density around Y01 A 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 Y01 B 402:

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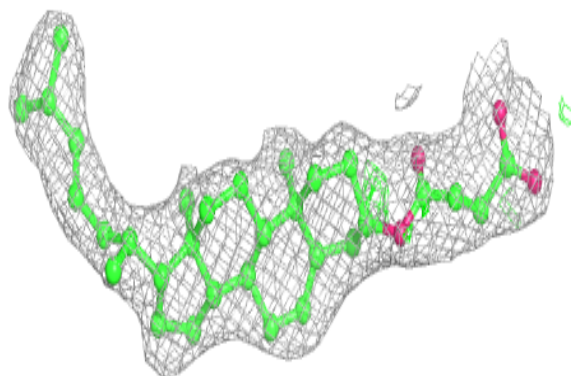and green (positive)

Electron density around Y00 A 601:

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

Electron density around Y01 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.