Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 04:23 pm BST

PDB ID	:	2BIW
Title	:	Crystal structure of apocarotenoid cleavage oxygenase from Synechocystis, native enzyme
Authors	:	Kloer, D.P.; Ruch, S.; Al-Babili, S.; Beyer, P.; Schulz, G.E.
Deposited on	:	2005-01-26
Resolution	:	2.39 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 following versions of software and data (see references ⓘ) were used in the production of this report:

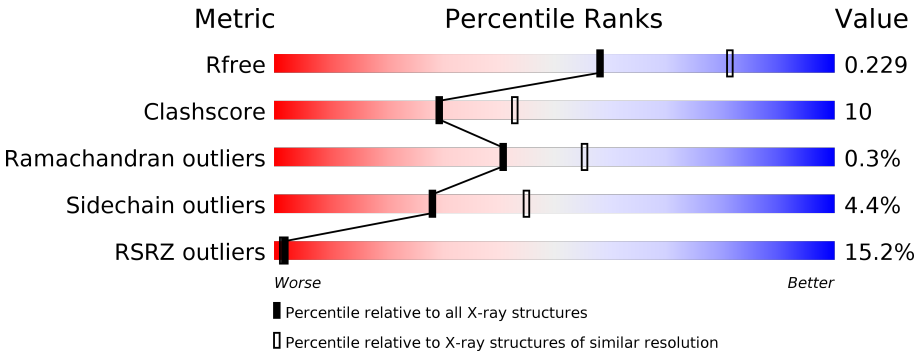
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.39 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	490	11% 78% 19%
1	B	490	13% 79% 18%
1	C	490	18% 79% 17%
1	D	490	18% 77% 19%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3ON	A	1491	-	-	-	X
2	3ON	B	1491	-	-	-	X
2	3ON	C	1491	-	-	-	X
2	3ON	D	1491	-	-	-	X

2 Entry composition

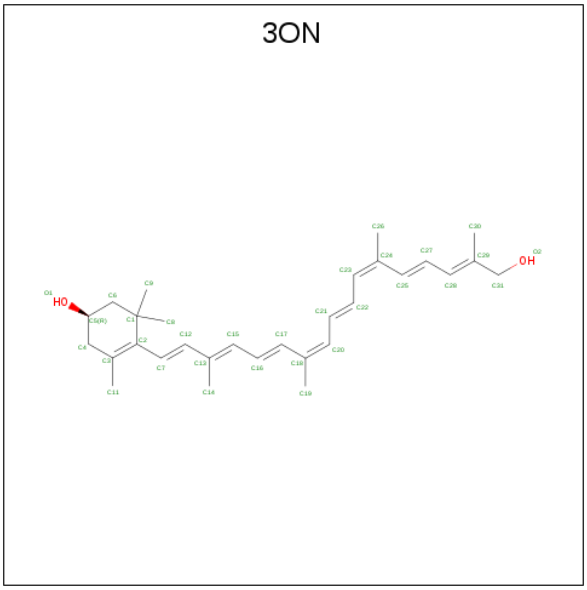
There are 4 unique types of molecules in this entry. The entry contains 15742 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 APOCAROTENOID-CLEAVING OXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3767	2417	650	690	10			
1	B	479	Total	C	N	O	S	0	0	0
			3767	2417	650	690	10			
1	C	479	Total	C	N	O	S	0	0	0
			3767	2417	650	690	10			
1	D	479	Total	C	N	O	S	0	0	0
			3767	2417	650	690	10			

- Molecule 2 is (3R)-3-HYDROXY-8'-APOCAROTENOL (three-letter code: 3ON) (formula: $C_{30}H_{42}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			32	30	2		
2	B	1	Total	C	O	0	0
			32	30	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 32 30 2	0	0
2	D	1	Total C O 32 30 2	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Fe 1 1	0	0
3	A	1	Total Fe 1 1	0	0
3	D	1	Total Fe 1 1	0	0
3	C	1	Total Fe 1 1	0	0

- Molecule 4 is water.

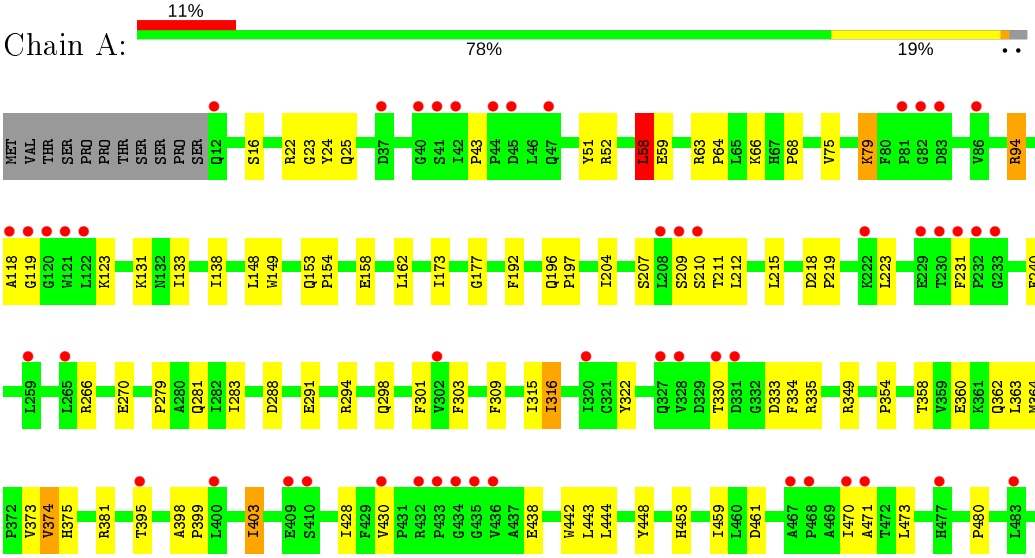
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	156	Total O 156 156	0	0
4	B	144	Total O 144 144	0	0
4	C	121	Total O 121 121	0	0
4	D	121	Total O 121 121	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

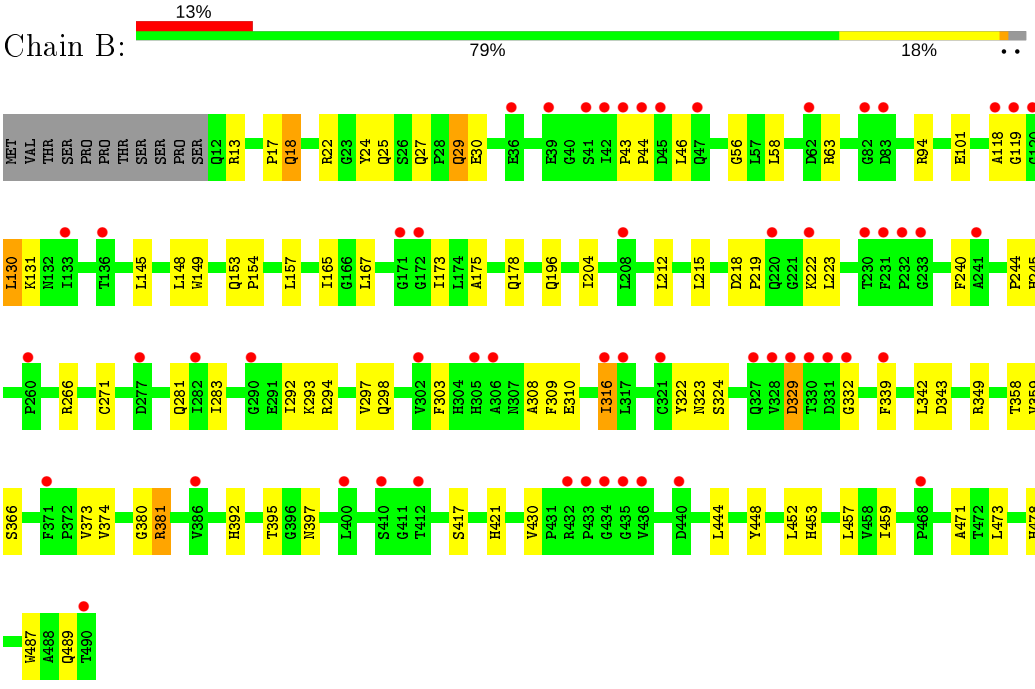
- Molecule 1: APOCAROTENOID-CLEAVING OXYGENASE

Chain A:



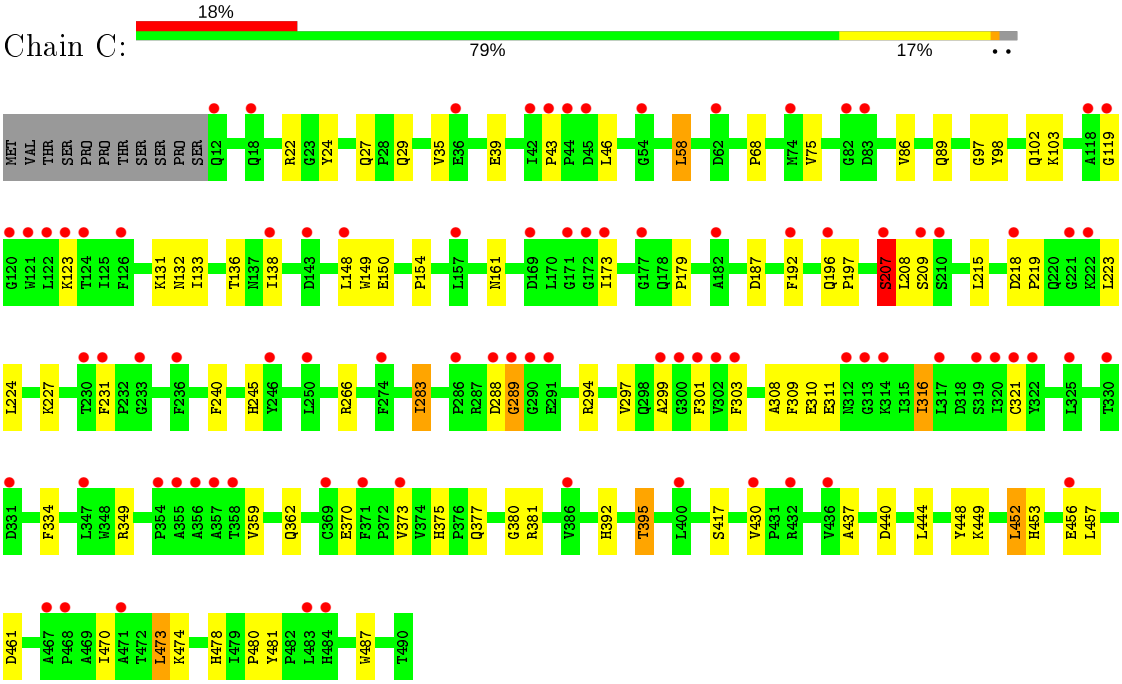
- Molecule 1: APOCAROTENOID-CLEAVING OXYGENASE

Chain B:



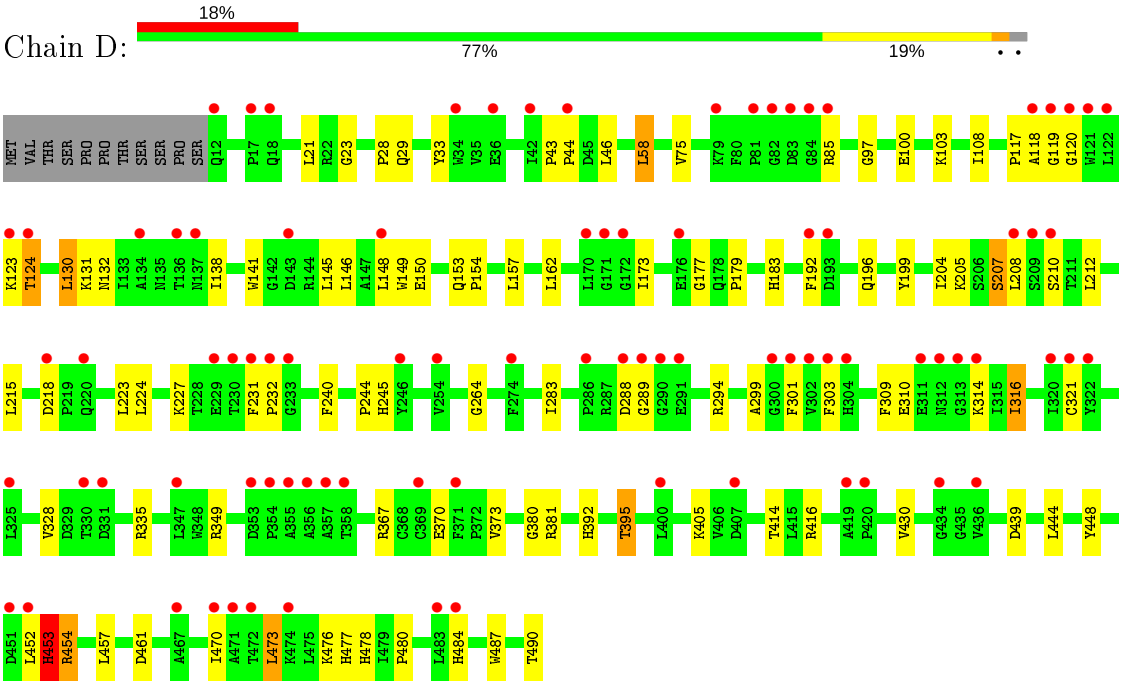
• Molecule 1: APOCAROTENOID-CLEAVING OXYGENASE

Chain C:



• Molecule 1: APOCAROTENOID-CLEAVING OXYGENASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	119.05Å 125.28Å 203.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.41 – 2.39 43.76 – 2.39	Depositor EDS
% Data completeness (in resolution range)	97.9 (44.41-2.39) 97.4 (43.76-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.180 , 0.224 0.187 , 0.229	Depositor DCC
R_{free} test set	5864 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 58.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.047 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15742	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, 3ON

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	0.75	0/3880	0.78	4/5285 (0.1%)
1	B	0.73	0/3880	0.77	2/5284 (0.0%)
1	C	0.68	0/3880	0.74	4/5284 (0.1%)
1	D	0.68	1/3880 (0.0%)	0.75	5/5284 (0.1%)
All	All	0.71	1/15520 (0.0%)	0.76	15/21137 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	85	ARG	NE-CZ	5.53	1.40	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	58	LEU	CA-CB-CG	-7.67	97.67	115.30
1	D	299	ALA	C-N-CA	-6.76	108.10	122.30
1	C	283	ILE	CG1-CB-CG2	-6.73	96.60	111.40
1	A	58	LEU	CA-CB-CG	-6.52	100.29	115.30
1	A	374	VAL	CG1-CB-CG2	6.16	120.75	110.90
1	C	299	ALA	C-N-CA	-6.13	109.42	122.30
1	D	130	LEU	CA-CB-CG	5.84	128.72	115.30
1	B	381	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	381	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	395	THR	C-N-CA	-5.51	110.72	122.30
1	D	395	THR	C-N-CA	-5.49	110.77	122.30
1	B	130	LEU	CB-CG-CD2	-5.46	101.72	111.00
1	C	58	LEU	CA-CB-CG	-5.28	103.15	115.30
1	D	453	HIS	N-CA-C	-5.20	96.97	111.00
1	A	395	THR	C-N-CA	-5.18	111.43	122.30

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	A	3767	0	3659	68	0
1	B	3767	0	3659	72	0
1	C	3767	0	3659	60	0
1	D	3767	0	3659	71	0
2	A	32	0	42	14	0
2	B	32	0	42	16	0
2	C	32	0	42	9	0
2	D	32	0	42	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	156	0	0	8	0
4	B	144	0	0	10	0
4	C	121	0	0	2	0
4	D	121	0	0	2	0
All	All	15742	0	14804	286	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 10.

All (286) 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:1491:3ON:H25	4:B:2022:HOH:O	1.52	1.10
2:D:1491:3ON:H28	4:D:2005:HOH:O	1.50	1.09
2:A:1491:3ON:H25	4:A:2035:HOH:O	1.52	1.08
2:C:1491:3ON:H25	4:C:2042:HOH:O	1.66	0.96
2:A:1491:3ON:H28	4:A:2008:HOH:O	1.65	0.95
1:D:46:LEU:HD12	1:D:430:VAL:HG11	1.54	0.90
1:A:281:GLN:NE2	1:A:294:ARG:HD3	1.89	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ARG:HH12	1:D:29:GLN:HE21	1.22	0.83
2:D:1491:3ON:H12	2:D:1491:3ON:H8C1	1.62	0.81
1:C:448:TYR:OH	1:C:453:HIS:HD2	1.64	0.80
1:C:449:LYS:HG2	1:C:456:GLU:OE1	1.83	0.79
1:D:454:ARG:CG	1:D:454:ARG:HH11	1.96	0.79
1:A:24:TYR:O	1:A:58:LEU:HD13	1.82	0.78
1:B:303:PHE:CD2	2:B:1491:3ON:H262	2.17	0.78
1:A:430:VAL:HG12	1:A:487:TRP:CG	2.17	0.78
1:B:130:LEU:HD21	2:B:1491:3ON:H113	1.66	0.77
1:D:303:PHE:CD2	2:D:1491:3ON:H263	2.20	0.77
1:D:370:GLU:HG3	2:D:1491:3ON:H302	1.67	0.77
1:D:454:ARG:HG3	1:D:454:ARG:HH11	1.51	0.75
1:B:430:VAL:HG21	1:B:444:LEU:HD11	1.69	0.74
1:A:281:GLN:HE22	1:A:294:ARG:HD3	1.49	0.74
1:A:211:THR:HG22	4:A:2081:HOH:O	1.87	0.74
1:B:448:TYR:OH	1:B:453:HIS:HD2	1.71	0.73
1:C:303:PHE:CD2	2:C:1491:3ON:H262	2.24	0.73
1:B:430:VAL:HG13	1:B:487:TRP:NE1	2.04	0.71
1:D:430:VAL:HG21	1:D:444:LEU:HD11	1.70	0.71
1:D:303:PHE:CD2	2:D:1491:3ON:C26	2.74	0.71
1:A:315:ILE:HD12	1:A:354:PRO:HG3	1.72	0.71
2:B:1491:3ON:H8C3	4:B:2075:HOH:O	1.91	0.70
1:C:309:PHE:CZ	1:C:316:ILE:HG12	2.27	0.69
1:A:333:ASP:OD2	1:A:335:ARG:NH1	2.25	0.69
1:A:430:VAL:HG11	1:A:444:LEU:HD11	1.74	0.69
1:B:204:ILE:HD12	1:B:212:LEU:HD12	1.72	0.69
1:A:153:GLN:NE2	1:A:177:GLY:H	1.91	0.69
1:B:245:HIS:HD2	1:B:310:GLU:OE1	1.76	0.67
1:A:430:VAL:HG12	1:A:487:TRP:CD2	2.29	0.67
1:A:283:ILE:HD13	1:A:294:ARG:HG2	1.76	0.67
1:A:448:TYR:OH	1:A:453:HIS:HD2	1.77	0.66
1:B:149:TRP:CZ2	2:B:1491:3ON:H142	2.30	0.66
1:B:281:GLN:HG3	1:B:294:ARG:NH2	2.09	0.66
1:B:24:TYR:O	1:B:58:LEU:HD22	1.95	0.66
1:D:46:LEU:CD1	1:D:430:VAL:HG11	2.25	0.66
1:C:24:TYR:O	1:C:58:LEU:HD13	1.95	0.66
1:A:430:VAL:CG2	1:A:442:TRP:HB2	2.24	0.66
1:A:173:ILE:CD1	1:A:223:LEU:HB2	2.24	0.66
1:C:370:GLU:HG3	2:C:1491:3ON:H302	1.75	0.66
1:D:448:TYR:OH	1:D:453:HIS:HD2	1.79	0.65
1:C:430:VAL:HG13	1:C:487:TRP:NE1	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ARG:HH21	1:B:271:CYS:HA	1.61	0.65
1:B:324:SER:OG	1:B:343:ASP:OD2	2.14	0.65
1:B:360:GLU:OE2	4:B:2107:HOH:O	2.14	0.65
1:C:316:ILE:HD13	1:C:349:ARG:NE	2.12	0.64
1:A:148:LEU:HD23	1:A:154:PRO:HB3	1.80	0.64
1:C:303:PHE:CG	2:C:1491:3ON:H262	2.34	0.63
1:D:204:ILE:HD12	1:D:212:LEU:HD12	1.81	0.63
1:D:309:PHE:CZ	1:D:316:ILE:HG12	2.33	0.62
1:A:210:SER:HB3	1:A:231:PHE:CZ	2.35	0.62
1:B:297:VAL:HB	1:B:359:VAL:HG11	1.82	0.62
1:A:281:GLN:OE1	1:A:283:ILE:HD11	1.99	0.61
1:A:298:GLN:HG3	1:B:30:GLU:O	1.99	0.61
1:B:392:HIS:HD2	1:B:417:SER:OG	1.83	0.61
1:C:392:HIS:HD2	1:C:417:SER:OG	1.84	0.61
2:B:1491:3ON:H12	2:B:1491:3ON:H9C1	1.82	0.61
1:D:405:LYS:NZ	1:D:439:ASP:OD2	2.30	0.60
1:B:46:LEU:HD12	1:B:430:VAL:HG11	1.83	0.60
1:B:145:LEU:HD23	1:B:157:LEU:HB2	1.83	0.60
1:C:303:PHE:CD2	2:C:1491:3ON:C26	2.85	0.60
1:A:43:PRO:HG3	1:A:470:ILE:HG21	1.84	0.59
1:D:430:VAL:CG2	1:D:444:LEU:HD11	2.33	0.59
1:A:316:ILE:HD13	1:A:349:ARG:NE	2.18	0.58
1:B:153:GLN:HB2	1:B:167:LEU:HD22	1.86	0.57
2:B:1491:3ON:H303	4:B:2042:HOH:O	2.03	0.57
1:A:430:VAL:HG12	1:A:487:TRP:CD1	2.38	0.57
1:D:153:GLN:NE2	1:D:177:GLY:H	2.01	0.57
1:B:119:GLY:HA3	1:B:123:LYS:HG3	1.85	0.57
1:C:227:LYS:NZ	1:C:289:GLY:HA2	2.20	0.57
1:C:136:THR:OG1	2:C:1491:3ON:H193	2.04	0.57
1:A:79:LYS:HB2	1:A:79:LYS:NZ	2.19	0.56
1:C:430:VAL:HG21	1:C:444:LEU:HD11	1.87	0.56
1:A:173:ILE:HD12	1:A:223:LEU:HB2	1.86	0.56
1:B:46:LEU:CD1	1:B:430:VAL:HG11	2.36	0.56
1:B:309:PHE:CZ	1:B:316:ILE:HG12	2.40	0.56
1:B:316:ILE:HD12	1:B:316:ILE:C	2.26	0.56
1:B:173:ILE:HD12	1:B:223:LEU:HB2	1.88	0.56
1:D:303:PHE:CG	2:D:1491:3ON:H262	2.40	0.56
1:A:309:PHE:CZ	1:A:316:ILE:HG12	2.40	0.55
1:C:448:TYR:OH	1:C:453:HIS:CD2	2.54	0.55
1:B:18:GLN:HE22	1:D:28:PRO:HB3	1.71	0.55
1:B:18:GLN:H	1:B:18:GLN:HE21	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:TRP:CE2	2:A:1491:3ON:H142	2.41	0.55
1:A:303:PHE:CG	2:A:1491:3ON:H262	2.42	0.55
1:C:449:LYS:O	1:C:452:LEU:O	2.23	0.55
1:A:196:GLN:HG3	1:A:197:PRO:HD2	1.88	0.55
1:C:187:ASP:OD1	1:C:381:ARG:NH2	2.40	0.55
1:D:430:VAL:HG22	1:D:487:TRP:CG	2.42	0.55
1:C:89:GLN:HE22	1:C:161:ASN:HA	1.72	0.54
1:D:119:GLY:HA3	1:D:123:LYS:HG3	1.89	0.54
2:A:1491:3ON:H6C1	4:A:2084:HOH:O	2.07	0.54
1:A:153:GLN:HE21	1:A:177:GLY:H	1.54	0.54
1:B:308:ALA:HA	1:B:316:ILE:O	2.07	0.54
1:D:454:ARG:CG	1:D:454:ARG:NH1	2.63	0.54
1:B:303:PHE:CD2	2:B:1491:3ON:C26	2.87	0.54
1:C:375:HIS:CE1	1:C:377:GLN:HG2	2.43	0.54
1:D:245:HIS:HD2	1:D:310:GLU:OE1	1.90	0.54
1:A:303:PHE:CD1	2:A:1491:3ON:H23	2.43	0.54
1:B:322:TYR:OH	2:B:1491:3ON:H302	2.08	0.54
1:A:210:SER:HB3	1:A:231:PHE:CE2	2.43	0.54
1:C:283:ILE:HG23	1:C:294:ARG:HG2	1.90	0.54
1:D:316:ILE:HD13	1:D:349:ARG:CD	2.38	0.54
1:D:119:GLY:HA3	1:D:123:LYS:CG	2.38	0.54
1:C:46:LEU:CD1	1:C:430:VAL:HG11	2.37	0.53
2:A:1491:3ON:H12	2:A:1491:3ON:H8C1	1.89	0.53
1:A:430:VAL:HG23	1:A:442:TRP:HE3	1.73	0.53
1:D:448:TYR:OH	1:D:453:HIS:CD2	2.60	0.53
1:B:149:TRP:CE2	2:B:1491:3ON:H142	2.43	0.53
1:B:25:GLN:O	1:B:478:HIS:HE1	1.92	0.53
1:A:149:TRP:CZ2	2:A:1491:3ON:H142	2.44	0.52
1:B:298:GLN:NE2	4:B:2090:HOH:O	2.42	0.52
1:C:218:ASP:HB2	1:C:219:PRO:CD	2.39	0.52
1:C:375:HIS:HE1	1:C:377:GLN:HG2	1.74	0.52
1:A:66:LYS:NZ	1:A:270:GLU:OE2	2.40	0.52
1:A:281:GLN:NE2	1:A:294:ARG:CD	2.68	0.52
1:A:303:PHE:CD2	2:A:1491:3ON:H262	2.45	0.52
1:B:22:ARG:HG2	1:B:453:HIS:CD2	2.45	0.52
2:A:1491:3ON:C12	2:A:1491:3ON:H8C1	2.40	0.52
1:A:461:ASP:HB2	1:A:470:ILE:HD11	1.90	0.52
1:D:430:VAL:HG22	1:D:487:TRP:CD2	2.44	0.52
1:D:303:PHE:CG	2:D:1491:3ON:C26	2.92	0.51
1:D:283:ILE:CD1	1:D:294:ARG:HE	2.23	0.51
1:C:457:LEU:HD23	1:C:473:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1491:3ON:H8C3	4:A:2084:HOH:O	2.09	0.51
1:D:218:ASP:HB3	1:D:224:LEU:HD21	1.92	0.51
1:B:56:GLY:HA2	1:B:480:PRO:HG2	1.92	0.51
1:B:218:ASP:HB2	1:B:219:PRO:CD	2.41	0.50
1:C:192:PHE:CE1	1:C:288:ASP:HB3	2.45	0.50
1:D:316:ILE:HD13	1:D:349:ARG:NE	2.26	0.50
1:C:218:ASP:HB2	1:C:219:PRO:HD2	1.93	0.50
1:D:75:VAL:HG12	1:D:162:LEU:HD13	1.94	0.50
1:D:303:PHE:CD2	2:D:1491:3ON:H262	2.46	0.50
1:D:118:ALA:O	1:D:123:LYS:HG3	2.12	0.49
1:A:291:GLU:OE1	1:A:291:GLU:HA	2.11	0.49
1:D:210:SER:HB3	1:D:231:PHE:CZ	2.47	0.49
1:C:119:GLY:HA3	1:C:123:LYS:HG3	1.94	0.49
1:D:192:PHE:CE1	1:D:288:ASP:HB3	2.48	0.49
1:B:489:GLN:NE2	4:B:2144:HOH:O	2.46	0.49
1:D:245:HIS:CD2	1:D:310:GLU:OE1	2.65	0.49
1:B:27:GLN:HE21	1:B:29:GLN:H	1.60	0.49
1:D:179:PRO:HD3	1:D:205:LYS:HE3	1.95	0.49
1:C:97:GLY:HA3	1:C:131:LYS:HG3	1.94	0.49
1:A:204:ILE:HD12	1:A:212:LEU:HD12	1.96	0.48
1:A:316:ILE:C	1:A:316:ILE:HD12	2.33	0.48
1:C:245:HIS:HD2	1:C:310:GLU:OE1	1.96	0.48
1:B:13:ARG:HH12	1:D:29:GLN:NE2	2.02	0.48
1:C:39:GLU:OE1	1:C:474:LYS:HD2	2.13	0.48
1:C:196:GLN:HG3	1:C:197:PRO:HD2	1.94	0.48
1:B:17:PRO:HD2	1:D:28:PRO:HB2	1.96	0.48
1:D:148:LEU:HD23	1:D:154:PRO:HB3	1.95	0.48
1:B:149:TRP:CE2	2:B:1491:3ON:C14	2.96	0.47
1:B:63:ARG:HH11	1:B:118:ALA:HB2	1.79	0.47
1:B:430:VAL:CG1	4:B:2144:HOH:O	2.62	0.47
1:A:100:GLU:OE1	1:A:109:TYR:OH	2.26	0.47
1:D:150:GLU:O	1:D:179:PRO:HB3	2.14	0.47
1:B:25:GLN:O	1:B:478:HIS:CE1	2.68	0.47
1:D:303:PHE:CE2	2:D:1491:3ON:H263	2.48	0.47
1:A:204:ILE:HA	1:A:211:THR:O	2.15	0.47
1:A:22:ARG:HG2	1:A:453:HIS:CD2	2.50	0.47
1:A:68:PRO:HD3	1:A:334:PHE:CD2	2.50	0.47
1:B:430:VAL:HG22	1:B:487:TRP:CG	2.50	0.47
1:B:316:ILE:HD13	1:B:349:ARG:HG3	1.96	0.47
1:B:342:LEU:HB2	1:B:397:ASN:ND2	2.30	0.46
1:A:375:HIS:HD2	1:A:438:GLU:O	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:LEU:HD21	1:D:335:ARG:HA	1.97	0.46
1:A:75:VAL:HG12	1:A:162:LEU:HD13	1.98	0.46
1:C:119:GLY:HA3	1:C:123:LYS:CG	2.45	0.46
1:D:227:LYS:NZ	1:D:289:GLY:HA2	2.31	0.46
1:C:27:GLN:HE21	1:C:29:GLN:H	1.62	0.46
2:C:1491:3ON:H22	4:C:2042:HOH:O	2.15	0.46
1:D:430:VAL:HG13	1:D:487:TRP:NE1	2.31	0.46
1:B:457:LEU:HD23	1:B:473:LEU:HD22	1.98	0.46
1:B:459:ILE:HD12	1:B:471:ALA:HB3	1.98	0.46
1:C:207:SER:OG	1:C:208:LEU:N	2.48	0.46
1:C:227:LYS:HZ3	1:C:289:GLY:HA2	1.80	0.46
1:B:430:VAL:HG21	1:B:444:LEU:CD1	2.43	0.45
2:C:1491:3ON:H261	2:C:1491:3ON:H27	1.43	0.45
1:A:22:ARG:HG3	1:A:25:GLN:NE2	2.32	0.45
1:A:430:VAL:HG23	1:A:430:VAL:O	2.16	0.45
1:B:218:ASP:OD2	1:B:222:LYS:HB2	2.16	0.45
1:B:43:PRO:HA	1:B:44:PRO:HD3	1.89	0.45
1:D:210:SER:HB2	1:D:231:PHE:CE1	2.52	0.45
1:D:132:ASN:HA	1:D:149:TRP:CZ3	2.51	0.45
1:B:244:PRO:HD3	1:B:380:GLY:O	2.17	0.45
1:C:309:PHE:CZ	1:C:316:ILE:CG1	2.99	0.45
1:D:303:PHE:CB	2:D:1491:3ON:H262	2.47	0.45
1:B:303:PHE:CG	2:B:1491:3ON:H262	2.51	0.45
1:B:175:ALA:O	1:B:178:GLN:HB3	2.16	0.45
1:C:43:PRO:HG3	1:C:470:ILE:HG21	1.98	0.45
1:B:303:PHE:CD1	2:B:1491:3ON:H23	2.51	0.45
2:B:1491:3ON:H6C1	4:B:2075:HOH:O	2.16	0.44
1:C:173:ILE:HD12	1:C:223:LEU:HB2	1.99	0.44
1:C:132:ASN:HA	1:C:149:TRP:CZ3	2.53	0.44
1:A:52:ARG:NH2	1:A:428:ILE:HG12	2.32	0.44
1:B:119:GLY:HA3	1:B:123:LYS:CG	2.48	0.44
1:C:136:THR:OG1	2:C:1491:3ON:C19	2.66	0.44
1:C:35:VAL:HB	1:C:86:VAL:HG13	2.00	0.44
1:C:461:ASP:HB2	1:C:470:ILE:HD11	1.98	0.44
1:A:430:VAL:HG23	1:A:442:TRP:HB2	1.99	0.44
1:B:18:GLN:HE21	1:B:18:GLN:N	2.14	0.44
1:C:297:VAL:HB	1:C:359:VAL:HG11	1.99	0.44
1:C:218:ASP:HB3	1:C:224:LEU:HD21	1.98	0.44
1:A:398:ALA:HB1	1:A:399:PRO:HD2	2.00	0.43
1:D:461:ASP:HB2	1:D:470:ILE:HD11	2.00	0.43
1:A:119:GLY:HA3	1:A:123:LYS:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ILE:HD13	1:B:349:ARG:NE	2.32	0.43
1:D:138:ILE:HA	1:D:146:LEU:O	2.17	0.43
1:D:141:TRP:CE2	1:D:199:TYR:HB2	2.53	0.43
1:A:298:GLN:CG	1:B:30:GLU:O	2.64	0.43
1:A:192:PHE:CE1	1:A:288:ASP:HB3	2.53	0.43
1:C:301:PHE:O	1:C:321:CYS:HA	2.18	0.43
1:D:173:ILE:HD12	1:D:223:LEU:HD22	2.00	0.43
1:A:131:LYS:HE3	1:A:133:ILE:CG2	2.48	0.43
1:B:283:ILE:HG23	1:B:292:ILE:CG2	2.49	0.43
1:B:18:GLN:HE22	1:D:28:PRO:CB	2.32	0.43
1:B:309:PHE:CZ	1:B:316:ILE:CG1	3.02	0.43
2:D:1491:3ON:H12	2:D:1491:3ON:C8	2.43	0.43
1:D:43:PRO:HA	1:D:44:PRO:HD3	1.95	0.43
1:D:124:THR:OG1	1:D:264:GLY:CA	2.67	0.43
1:D:23:GLY:O	1:D:480:PRO:HA	2.17	0.43
1:A:63:ARG:HD2	1:A:118:ALA:HB2	2.01	0.43
2:A:1491:3ON:C28	4:A:2008:HOH:O	2.42	0.43
1:D:244:PRO:HD3	1:D:380:GLY:O	2.19	0.43
1:B:309:PHE:CE2	1:B:316:ILE:HG13	2.54	0.42
1:A:59:GLU:CB	1:A:64:PRO:HA	2.49	0.42
1:C:308:ALA:O	1:C:380:GLY:HA2	2.19	0.42
2:D:1491:3ON:H25	4:D:2005:HOH:O	2.18	0.42
1:A:363:LEU:HD21	1:A:366:SER:HB3	2.01	0.42
1:A:430:VAL:CG1	1:A:444:LEU:HD11	2.45	0.42
1:C:75:VAL:HG11	1:C:138:ILE:CD1	2.50	0.42
1:C:480:PRO:O	1:C:481:TYR:C	2.58	0.42
1:A:459:ILE:HD12	1:A:471:ALA:HB3	2.00	0.42
1:B:165:ILE:HD13	1:B:165:ILE:N	2.35	0.42
1:C:148:LEU:HD23	1:C:154:PRO:HB3	2.00	0.42
1:C:437:ALA:HB3	1:C:440:ASP:HB2	2.02	0.42
1:C:98:TYR:O	1:C:102:GLN:HG2	2.20	0.42
2:B:1491:3ON:H27	2:B:1491:3ON:H261	1.27	0.42
1:D:231:PHE:HA	1:D:232:PRO:HD3	1.95	0.42
1:A:403:ILE:HD11	1:A:443:LEU:CD1	2.50	0.41
1:C:430:VAL:HG21	1:C:444:LEU:CD1	2.50	0.41
1:D:108:ILE:O	1:D:117:PRO:HG3	2.20	0.41
1:D:367:ARG:NH1	1:D:392:HIS:O	2.48	0.41
2:A:1491:3ON:H141	2:A:1491:3ON:H16	1.92	0.41
1:A:218:ASP:HB2	1:A:219:PRO:CD	2.51	0.41
1:C:392:HIS:CD2	1:C:417:SER:OG	2.69	0.41
1:C:430:VAL:HG22	1:C:487:TRP:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:PHE:N	1:A:322:TYR:O	2.50	0.41
1:D:33:TYR:CE1	1:D:476:LYS:HD2	2.55	0.41
1:A:51:TYR:HB3	1:A:138:ILE:HD13	2.02	0.41
1:B:363:LEU:HD21	1:B:366:SER:HB3	2.01	0.41
1:C:22:ARG:HG2	1:C:453:HIS:CD2	2.55	0.41
1:C:309:PHE:CE2	1:C:316:ILE:CG1	3.04	0.41
1:D:207:SER:HB3	1:D:208:LEU:H	1.69	0.41
1:D:301:PHE:O	1:D:321:CYS:HA	2.20	0.41
1:D:97:GLY:HA3	1:D:131:LYS:HG3	2.03	0.41
1:B:101:GLU:OE1	1:B:131:LYS:NZ	2.42	0.41
1:B:329:ASP:OD2	1:B:332:GLY:HA3	2.20	0.41
1:C:131:LYS:HE3	1:C:133:ILE:CG2	2.50	0.41
1:A:430:VAL:CG1	1:A:487:TRP:CD2	3.02	0.41
1:B:323:ASN:ND2	4:B:2098:HOH:O	2.34	0.41
1:D:309:PHE:CZ	1:D:316:ILE:CG1	3.02	0.41
1:B:148:LEU:HD23	1:B:154:PRO:HB3	2.02	0.41
1:C:123:LYS:HD3	1:C:123:LYS:HA	1.90	0.41
1:D:477:HIS:HD2	1:D:478:HIS:O	2.04	0.41
2:A:1491:3ON:H27	2:A:1491:3ON:H261	1.36	0.41
1:B:421:HIS:CE1	4:B:2123:HOH:O	2.74	0.41
1:C:150:GLU:O	1:C:179:PRO:HB3	2.21	0.41
1:A:23:GLY:O	1:A:480:PRO:HA	2.20	0.40
1:A:298:GLN:HA	4:A:2102:HOH:O	2.21	0.40
1:A:94:ARG:NH2	4:A:2037:HOH:O	2.53	0.40
1:B:149:TRP:NE1	2:B:1491:3ON:H141	2.35	0.40
1:D:120:GLY:O	1:D:124:THR:HG23	2.21	0.40
1:D:173:ILE:HD12	1:D:223:LEU:HB2	2.03	0.40
1:D:145:LEU:HD23	1:D:157:LEU:HB2	2.03	0.40
1:D:457:LEU:HB3	1:D:473:LEU:HD22	2.03	0.40
1:C:68:PRO:HD3	1:C:334:PHE:CD2	2.57	0.40
1:D:183:HIS:HE1	1:D:484:HIS:CE1	2.39	0.40
1:D:210:SER:CB	1:D:231:PHE:CZ	3.04	0.40
1:A:403:ILE:HD11	1:A:443:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	477/490 (97%)	461 (97%)	15 (3%)	1 (0%)	47	62
1	B	477/490 (97%)	459 (96%)	17 (4%)	1 (0%)	47	62
1	C	477/490 (97%)	461 (97%)	14 (3%)	2 (0%)	34	48
1	D	477/490 (97%)	458 (96%)	17 (4%)	2 (0%)	34	48
All	All	1908/1960 (97%)	1839 (96%)	63 (3%)	6 (0%)	41	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	339	PHE
1	C	207	SER
1	D	452	LEU
1	D	453	HIS
1	A	330	THR
1	C	289	GLY

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	A	399/410 (97%)	379 (95%)	20 (5%)	24	40
1	B	399/410 (97%)	384 (96%)	15 (4%)	33	51
1	C	399/410 (97%)	384 (96%)	15 (4%)	33	51
1	D	399/410 (97%)	379 (95%)	20 (5%)	24	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1596/1640 (97%)	1526 (96%)	70 (4%)	28 45

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	58	LEU
1	A	79	LYS
1	A	94	ARG
1	A	158	GLU
1	A	207	SER
1	A	209	SER
1	A	215	LEU
1	A	240	PHE
1	A	266	ARG
1	A	279	PRO
1	A	316	ILE
1	A	358	THR
1	A	360	GLU
1	A	362	GLN
1	A	364	MET
1	A	373	VAL
1	A	374	VAL
1	A	403	ILE
1	A	473	LEU
1	B	18	GLN
1	B	29	GLN
1	B	94	ARG
1	B	196	GLN
1	B	215	LEU
1	B	240	PHE
1	B	293	LYS
1	B	316	ILE
1	B	329	ASP
1	B	358	THR
1	B	373	VAL
1	B	374	VAL
1	B	381	ARG
1	B	395	THR
1	B	452	LEU
1	C	103	LYS
1	C	207	SER

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Mol	Chain	Res	Type
1	C	209	SER
1	C	215	LEU
1	C	231	PHE
1	C	240	PHE
1	C	266	ARG
1	C	311	GLU
1	C	316	ILE
1	C	362	GLN
1	C	373	VAL
1	C	395	THR
1	C	452	LEU
1	C	473	LEU
1	C	478	HIS
1	D	58	LEU
1	D	100	GLU
1	D	103	LYS
1	D	124	THR
1	D	130	LEU
1	D	196	GLN
1	D	207	SER
1	D	215	LEU
1	D	240	PHE
1	D	314	LYS
1	D	316	ILE
1	D	328	VAL
1	D	373	VAL
1	D	381	ARG
1	D	395	THR
1	D	414	THR
1	D	416	ARG
1	D	454	ARG
1	D	473	LEU
1	D	490	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	29	GLN
1	A	153	GLN
1	A	245	HIS
1	A	453	HIS

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Mol	Chain	Res	Type
1	B	18	GLN
1	B	27	GLN
1	B	29	GLN
1	B	153	GLN
1	B	196	GLN
1	B	226	GLN
1	B	245	HIS
1	B	362	GLN
1	B	392	HIS
1	B	453	HIS
1	B	477	HIS
1	B	478	HIS
1	C	25	GLN
1	C	27	GLN
1	C	89	GLN
1	C	153	GLN
1	C	245	HIS
1	C	362	GLN
1	C	392	HIS
1	C	421	HIS
1	C	453	HIS
1	C	477	HIS
1	C	478	HIS
1	D	25	GLN
1	D	29	GLN
1	D	96	GLN
1	D	116	GLN
1	D	153	GLN
1	D	245	HIS
1	D	312	ASN
1	D	421	HIS
1	D	453	HIS
1	D	477	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
2	3ON	A	1491	-	31,32,32	1.25	4 (12%)	38,42,42	2.78	18 (47%)
2	3ON	D	1491	-	31,32,32	1.44	5 (16%)	38,42,42	2.53	11 (28%)
2	3ON	B	1491	-	31,32,32	1.27	1 (3%)	38,42,42	2.94	18 (47%)
2	3ON	C	1491	-	31,32,32	1.34	3 (9%)	38,42,42	2.43	13 (34%)

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
2	3ON	A	1491	-	-	7/26/45/45	0/1/1/1
2	3ON	D	1491	-	-	10/26/45/45	0/1/1/1
2	3ON	B	1491	-	-	9/26/45/45	0/1/1/1
2	3ON	C	1491	-	-	8/26/45/45	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1491	3ON	C1-C2	3.32	1.58	1.53
2	C	1491	3ON	C6-C5	2.90	1.56	1.52
2	D	1491	3ON	C1-C2	2.74	1.57	1.53
2	A	1491	3ON	C6-C5	2.56	1.56	1.52
2	B	1491	3ON	C20-C18	2.56	1.39	1.35
2	C	1491	3ON	C28-C29	2.47	1.36	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1491	3ON	C7-C2	2.44	1.53	1.45
2	D	1491	3ON	C28-C29	2.34	1.36	1.34
2	A	1491	3ON	C1-C2	2.25	1.56	1.53
2	A	1491	3ON	C28-C29	2.16	1.36	1.34
2	A	1491	3ON	C4-C5	2.14	1.55	1.52
2	D	1491	3ON	C23-C24	2.03	1.38	1.35
2	D	1491	3ON	C4-C3	2.00	1.54	1.51

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1491	3ON	C25-C24-C23	6.82	129.41	118.94
2	D	1491	3ON	C25-C24-C23	6.80	129.37	118.94
2	B	1491	3ON	C25-C24-C23	6.54	128.98	118.94
2	D	1491	3ON	C17-C18-C20	6.36	128.70	118.94
2	D	1491	3ON	C26-C24-C25	-6.30	108.14	118.08
2	C	1491	3ON	C17-C18-C20	6.24	128.51	118.94
2	B	1491	3ON	C1-C2-C3	-6.12	113.99	122.61
2	B	1491	3ON	C26-C24-C25	-5.96	108.69	118.08
2	C	1491	3ON	C25-C24-C23	5.41	127.25	118.94
2	A	1491	3ON	C22-C21-C20	-5.37	112.48	123.47
2	B	1491	3ON	C21-C22-C23	5.36	134.46	123.47
2	A	1491	3ON	C17-C18-C20	5.31	127.09	118.94
2	C	1491	3ON	C26-C24-C25	-5.06	110.11	118.08
2	C	1491	3ON	C1-C2-C3	-4.97	115.61	122.61
2	A	1491	3ON	C26-C24-C25	-4.91	110.35	118.08
2	B	1491	3ON	C17-C18-C20	4.90	126.46	118.94
2	B	1491	3ON	C22-C21-C20	-4.60	114.06	123.47
2	A	1491	3ON	C1-C2-C3	-4.58	116.16	122.61
2	A	1491	3ON	C21-C22-C23	4.55	132.80	123.47
2	C	1491	3ON	C19-C18-C20	-4.43	116.71	122.92
2	C	1491	3ON	C1-C2-C7	4.07	127.28	115.78
2	B	1491	3ON	C11-C3-C2	-4.02	120.01	124.53
2	D	1491	3ON	C19-C18-C20	-4.02	117.29	122.92
2	D	1491	3ON	C11-C3-C2	-3.79	120.27	124.53
2	C	1491	3ON	C9-C1-C2	3.77	116.42	110.30
2	D	1491	3ON	C9-C1-C2	3.68	116.27	110.30
2	B	1491	3ON	C19-C18-C17	-3.64	112.33	118.08
2	A	1491	3ON	C1-C6-C5	3.62	121.81	113.64
2	B	1491	3ON	C27-C25-C24	-3.49	116.61	126.42
2	B	1491	3ON	C14-C13-C15	-3.41	118.15	122.92
2	A	1491	3ON	C11-C3-C2	-3.37	120.74	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1491	3ON	C1-C2-C3	-3.37	117.87	122.61
2	B	1491	3ON	C11-C3-C4	3.34	120.55	114.36
2	A	1491	3ON	C1-C2-C7	3.28	125.06	115.78
2	D	1491	3ON	C1-C2-C7	3.20	124.83	115.78
2	B	1491	3ON	C1-C2-C7	3.20	124.83	115.78
2	A	1491	3ON	C27-C25-C24	-3.16	117.53	126.42
2	A	1491	3ON	C19-C18-C20	-3.10	118.58	122.92
2	B	1491	3ON	C1-C6-C5	3.09	120.62	113.64
2	B	1491	3ON	C21-C20-C18	-3.08	122.91	127.31
2	A	1491	3ON	C11-C3-C4	3.08	120.06	114.36
2	B	1491	3ON	C12-C13-C15	2.83	123.28	118.94
2	A	1491	3ON	C6-C5-C4	2.75	114.06	110.30
2	D	1491	3ON	C19-C18-C17	-2.59	114.00	118.08
2	D	1491	3ON	C28-C27-C25	-2.52	115.35	123.22
2	C	1491	3ON	C6-C5-C4	2.44	113.65	110.30
2	A	1491	3ON	C26-C24-C23	-2.42	119.54	122.92
2	A	1491	3ON	C19-C18-C17	-2.38	114.33	118.08
2	B	1491	3ON	C22-C23-C24	-2.38	123.92	127.31
2	C	1491	3ON	C11-C3-C4	2.37	118.75	114.36
2	D	1491	3ON	C21-C22-C23	2.36	128.30	123.47
2	A	1491	3ON	C14-C13-C15	-2.35	119.63	122.92
2	B	1491	3ON	C16-C15-C13	-2.34	123.98	127.31
2	C	1491	3ON	C22-C23-C24	-2.33	123.98	127.31
2	A	1491	3ON	C12-C13-C15	2.24	122.37	118.94
2	C	1491	3ON	C27-C25-C24	-2.22	120.18	126.42
2	A	1491	3ON	C21-C20-C18	-2.17	124.21	127.31
2	C	1491	3ON	C19-C18-C17	-2.10	114.77	118.08
2	B	1491	3ON	C6-C5-C4	2.08	113.15	110.30
2	C	1491	3ON	C15-C16-C17	-2.01	116.96	123.22

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1491	3ON	C30-C29-C31-O2
2	C	1491	3ON	C30-C29-C31-O2
2	A	1491	3ON	C30-C29-C31-O2
2	D	1491	3ON	C7-C12-C13-C14
2	D	1491	3ON	C7-C12-C13-C15
2	B	1491	3ON	C22-C23-C24-C25
2	B	1491	3ON	C18-C20-C21-C22
2	A	1491	3ON	C18-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
2	B	1491	3ON	C28-C29-C31-O2
2	A	1491	3ON	C28-C29-C31-O2
2	D	1491	3ON	C28-C29-C31-O2
2	A	1491	3ON	C22-C23-C24-C25
2	D	1491	3ON	C30-C29-C31-O2
2	C	1491	3ON	C21-C22-C23-C24
2	B	1491	3ON	C19-C18-C20-C21
2	B	1491	3ON	C22-C23-C24-C26
2	C	1491	3ON	C19-C18-C20-C21
2	C	1491	3ON	C22-C23-C24-C26
2	A	1491	3ON	C19-C18-C20-C21
2	A	1491	3ON	C22-C23-C24-C26
2	D	1491	3ON	C19-C18-C20-C21
2	D	1491	3ON	C22-C23-C24-C26
2	B	1491	3ON	C17-C18-C20-C21
2	C	1491	3ON	C17-C18-C20-C21
2	A	1491	3ON	C17-C18-C20-C21
2	D	1491	3ON	C17-C18-C20-C21
2	D	1491	3ON	C22-C23-C24-C25
2	C	1491	3ON	C1-C2-C7-C12
2	C	1491	3ON	C22-C23-C24-C25
2	B	1491	3ON	C3-C2-C7-C12
2	B	1491	3ON	C1-C2-C7-C12
2	C	1491	3ON	C3-C2-C7-C12
2	D	1491	3ON	C3-C2-C7-C12
2	D	1491	3ON	C1-C2-C7-C12

There are no ring outliers.

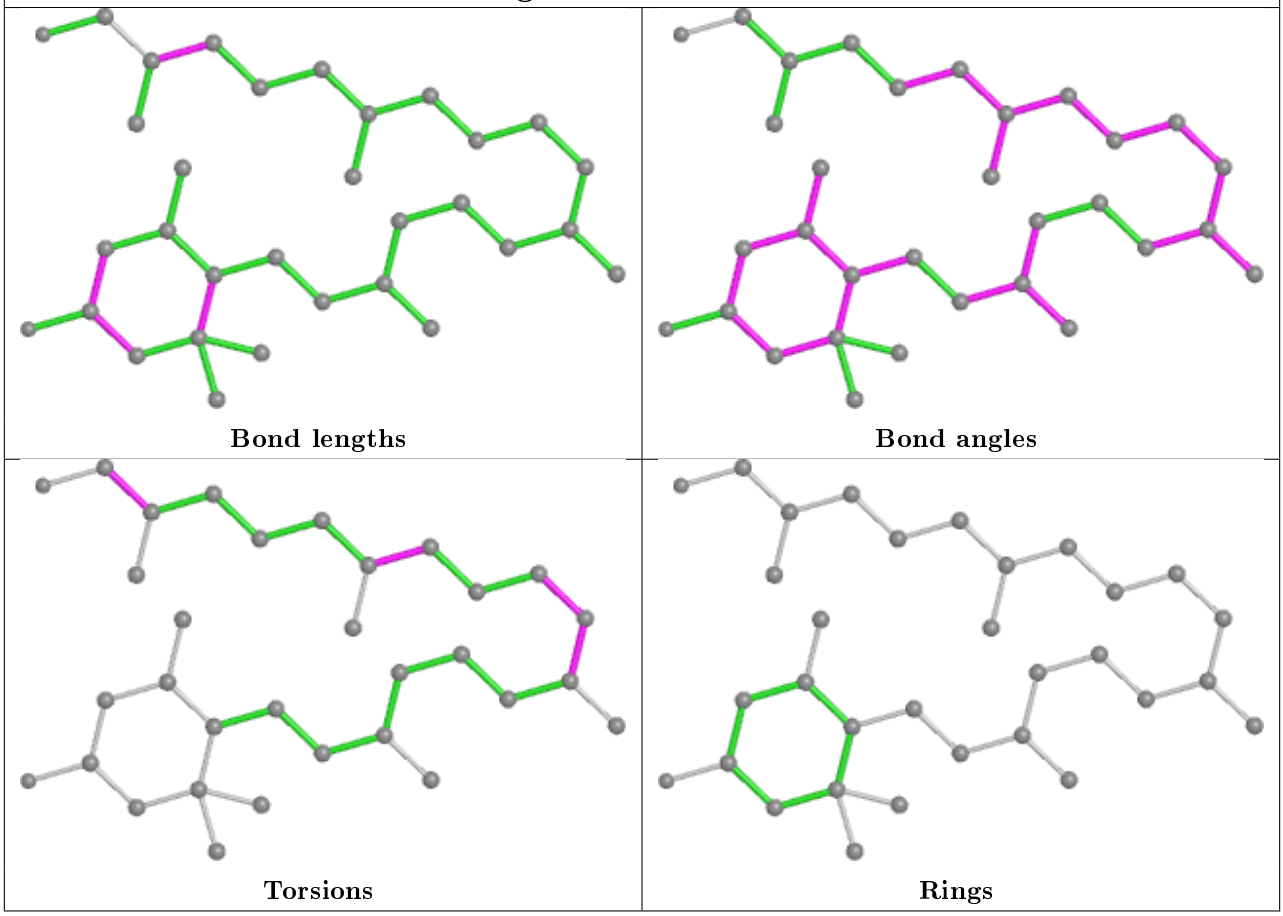
4 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1491	3ON	14	0
2	D	1491	3ON	12	0
2	B	1491	3ON	16	0
2	C	1491	3ON	9	0

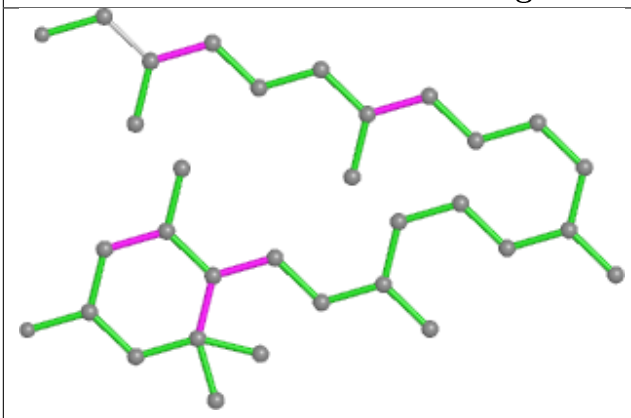
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

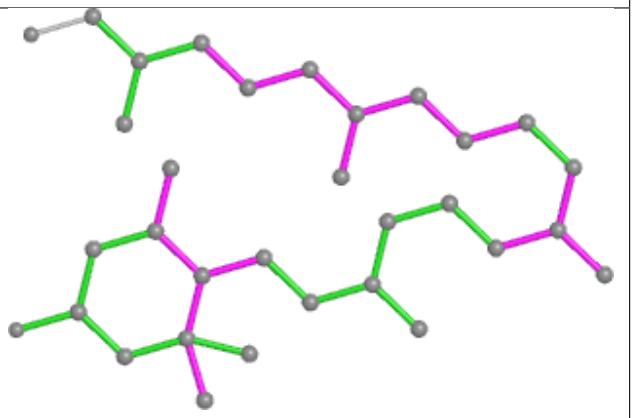
Ligand 3ON A 1491



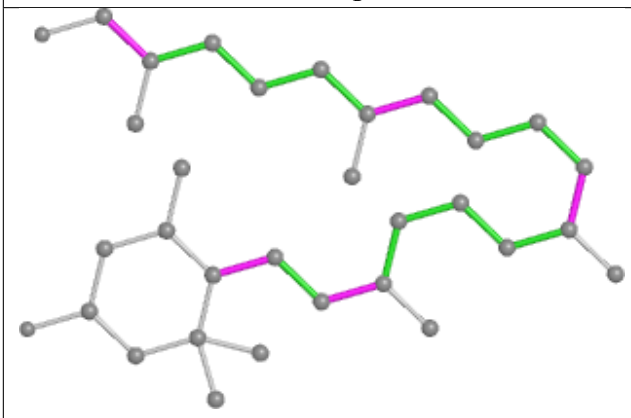
Ligand 3ON D 1491



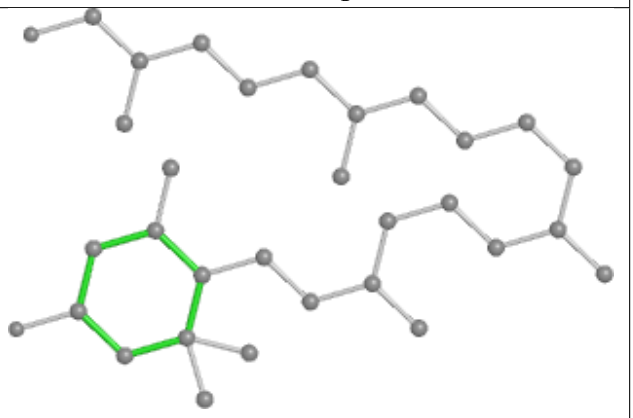
Bond lengths



Bond angles

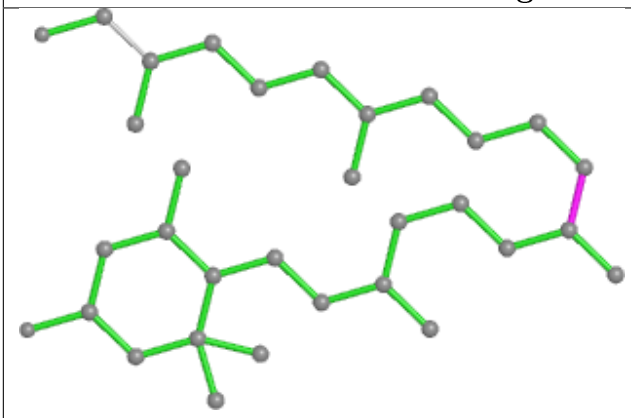


Torsions

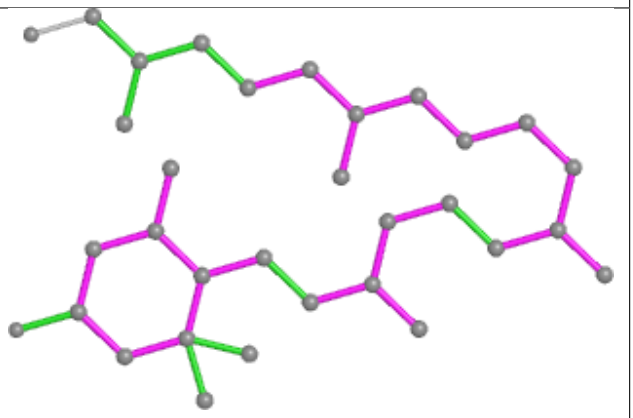


Rings

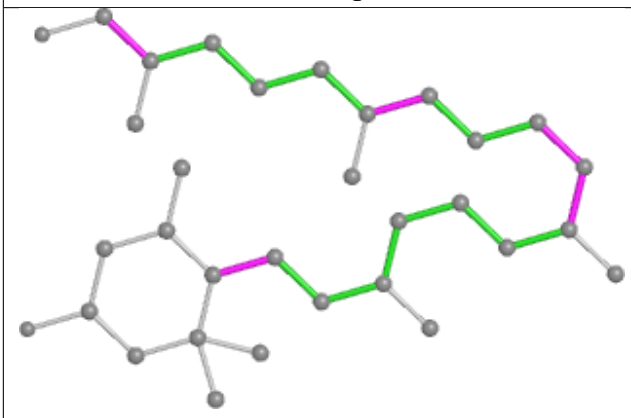
Ligand 3ON B 1491



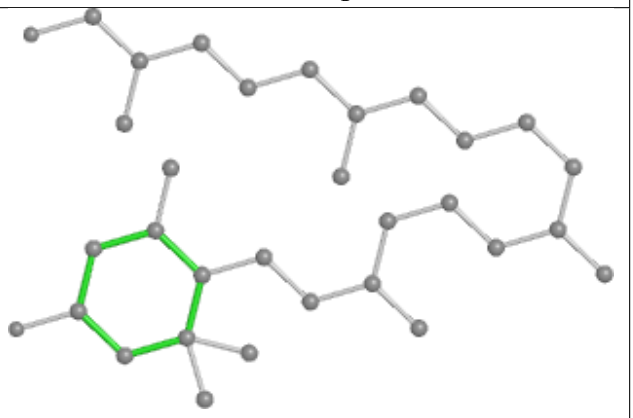
Bond lengths



Bond angles

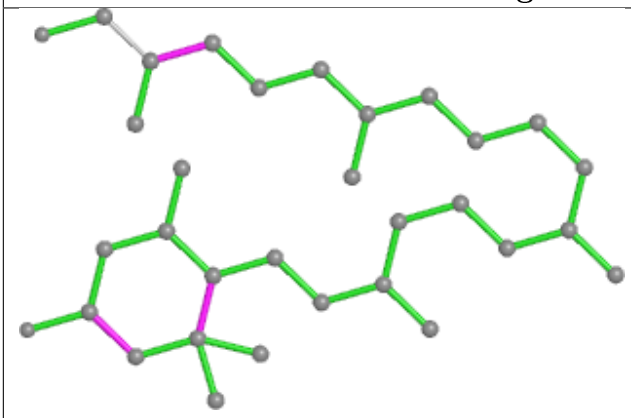


Torsions

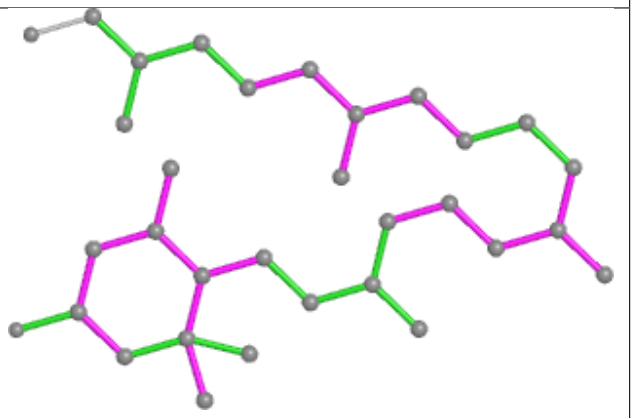


Rings

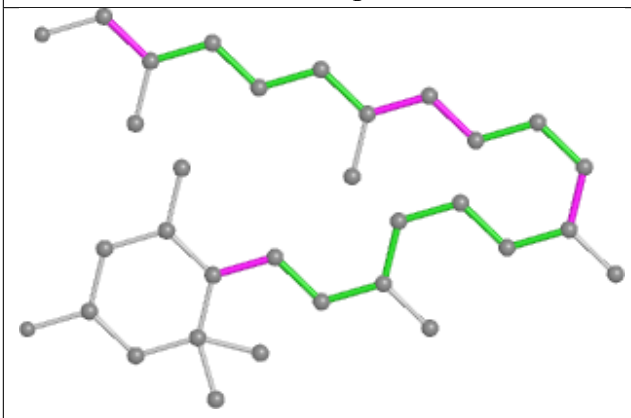
Ligand 3ON C 1491



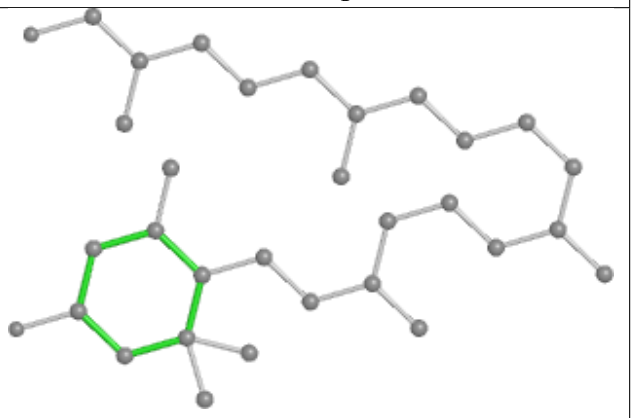
Bond lengths



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, 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	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	479/490 (97%)	0.95	55 (11%)	4 4	55, 63, 74, 86	0
1	B	479/490 (97%)	0.99	62 (12%)	3 3	54, 63, 74, 86	0
1	C	479/490 (97%)	1.20	86 (17%)	1 1	56, 63, 74, 86	0
1	D	479/490 (97%)	1.21	88 (18%)	1 1	55, 63, 74, 87	0
All	All	1916/1960 (97%)	1.09	291 (15%)	2 1	54, 63, 74, 87	0

All (291) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	THR	8.5
1	A	331	ASP	7.9
1	B	330	THR	7.9
1	D	121	TRP	6.5
1	A	232	PRO	6.4
1	A	208	LEU	6.3
1	C	436	VAL	6.3
1	B	121	TRP	6.2
1	C	119	GLY	6.2
1	D	233	GLY	6.1
1	C	121	TRP	6.1
1	C	230	THR	6.0
1	C	356	ALA	5.9
1	A	433	PRO	5.5
1	B	329	ASP	5.4
1	D	231	PHE	5.4
1	C	355	ALA	5.4
1	D	313	GLY	5.4
1	B	122	LEU	5.2
1	D	289	GLY	5.0
1	B	331	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	312	ASN	4.9
1	D	331	ASP	4.8
1	B	436	VAL	4.8
1	B	412	THR	4.8
1	C	289	GLY	4.7
1	D	467	ALA	4.7
1	C	118	ALA	4.6
1	D	312	ASN	4.6
1	A	328	VAL	4.6
1	D	355	ALA	4.6
1	B	328	VAL	4.5
1	C	171	GLY	4.5
1	B	208	LEU	4.5
1	D	357	ALA	4.4
1	A	120	GLY	4.4
1	D	83	ASP	4.4
1	D	232	PRO	4.4
1	B	62	ASP	4.4
1	A	121	TRP	4.4
1	D	356	ALA	4.3
1	C	120	GLY	4.3
1	D	171	GLY	4.3
1	B	327	GLN	4.3
1	B	232	PRO	4.2
1	D	288	ASP	4.2
1	D	122	LEU	4.2
1	D	483	LEU	4.2
1	D	436	VAL	4.2
1	D	434	GLY	4.1
1	A	122	LEU	4.1
1	C	371	PHE	4.1
1	D	44	PRO	4.0
1	D	176	GLU	4.0
1	D	12	GLN	4.0
1	A	231	PHE	4.0
1	C	290	GLY	3.9
1	D	118	ALA	3.9
1	D	192	PHE	3.9
1	A	42	ILE	3.9
1	D	18	GLN	3.9
1	C	483	LEU	3.9
1	D	82	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	330	THR	3.7
1	D	230	THR	3.7
1	D	371	PHE	3.7
1	A	434	GLY	3.7
1	D	314	LYS	3.7
1	C	218	ASP	3.7
1	C	291	GLU	3.6
1	C	45	ASP	3.6
1	C	320	ILE	3.6
1	C	357	ALA	3.6
1	C	172	GLY	3.5
1	B	43	PRO	3.5
1	D	302	VAL	3.5
1	C	233	GLY	3.5
1	C	358	THR	3.5
1	D	123	LYS	3.5
1	C	288	ASP	3.5
1	C	44	PRO	3.4
1	D	290	GLY	3.4
1	C	467	ALA	3.4
1	B	233	GLY	3.4
1	D	193	ASP	3.3
1	A	327	GLN	3.3
1	D	452	LEU	3.3
1	D	301	PHE	3.3
1	D	321	CYS	3.3
1	D	358	THR	3.3
1	D	320	ILE	3.3
1	A	490	THR	3.3
1	B	483	LEU	3.2
1	C	354	PRO	3.2
1	C	330	THR	3.2
1	D	209	SER	3.2
1	C	173	ILE	3.2
1	C	303	PHE	3.2
1	D	124	THR	3.2
1	D	347	LEU	3.2
1	A	47	GLN	3.2
1	A	44	PRO	3.2
1	B	230	THR	3.1
1	A	45	ASP	3.1
1	B	120	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	41	SER	3.1
1	C	209	SER	3.1
1	B	44	PRO	3.1
1	C	42	ILE	3.1
1	A	119	GLY	3.1
1	C	83	ASP	3.1
1	C	210	SER	3.1
1	C	322	TYR	3.1
1	C	148	LEU	3.0
1	B	82	GLY	3.0
1	C	456	GLU	3.0
1	A	483	LEU	3.0
1	B	435	GLY	3.0
1	C	236	PHE	3.0
1	D	120	GLY	3.0
1	A	468	PRO	3.0
1	C	124	THR	3.0
1	C	62	ASP	2.9
1	D	300	GLY	2.9
1	C	471	ALA	2.9
1	C	286	PRO	2.9
1	A	230	THR	2.9
1	C	143	ASP	2.9
1	B	171	GLY	2.9
1	B	490	THR	2.9
1	B	231	PHE	2.9
1	C	126	PHE	2.9
1	C	331	ASP	2.8
1	D	134	ALA	2.8
1	D	84	GLY	2.8
1	B	306	ALA	2.8
1	A	229	GLU	2.8
1	C	321	CYS	2.8
1	D	119	GLY	2.8
1	C	18	GLN	2.8
1	A	210	SER	2.8
1	C	432	ARG	2.8
1	C	182	ALA	2.8
1	C	314	LYS	2.8
1	D	451	ASP	2.8
1	C	123	LYS	2.8
1	D	143	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	229	GLU	2.8
1	D	208	LEU	2.7
1	A	470	ILE	2.7
1	C	246	TYR	2.7
1	A	430	VAL	2.7
1	D	303	PHE	2.7
1	C	250	LEU	2.7
1	B	118	ALA	2.7
1	C	301	PHE	2.7
1	A	395	THR	2.7
1	D	353	ASP	2.7
1	D	81	PRO	2.6
1	B	386	VAL	2.6
1	C	484	HIS	2.6
1	D	291	GLU	2.6
1	A	118	ALA	2.6
1	A	432	ARG	2.6
1	C	347	LEU	2.6
1	C	231	PHE	2.6
1	B	290	GLY	2.6
1	D	471	ALA	2.6
1	B	257	ASN	2.6
1	D	470	ILE	2.6
1	D	210	SER	2.5
1	A	259	LEU	2.5
1	D	274	PHE	2.5
1	B	119	GLY	2.5
1	A	400	LEU	2.5
1	D	218	ASP	2.5
1	A	371	PHE	2.5
1	B	302	VAL	2.5
1	D	254	VAL	2.5
1	A	12	GLN	2.5
1	B	248	ILE	2.5
1	B	172	GLY	2.5
1	B	41	SER	2.5
1	D	286	PRO	2.5
1	B	434	GLY	2.5
1	C	400	LEU	2.5
1	B	371	PHE	2.4
1	C	373	VAL	2.4
1	C	468	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	472	THR	2.4
1	B	45	ASP	2.4
1	C	207	SER	2.4
1	C	74	MET	2.4
1	A	467	ALA	2.4
1	C	12	GLN	2.4
1	D	420	PRO	2.4
1	B	317	LEU	2.4
1	C	169	ASP	2.4
1	A	81	PRO	2.4
1	D	136	THR	2.4
1	A	209	SER	2.4
1	D	220	GLN	2.4
1	C	386	VAL	2.4
1	C	369	CYS	2.4
1	C	313	GLY	2.3
1	C	36	GLU	2.3
1	C	82	GLY	2.3
1	B	123	LYS	2.3
1	B	433	PRO	2.3
1	C	325	LEU	2.3
1	B	136	THR	2.3
1	B	260	PRO	2.3
1	A	265	LEU	2.3
1	C	302	VAL	2.3
1	D	172	GLY	2.3
1	A	248	ILE	2.3
1	A	247	ALA	2.3
1	C	122	LEU	2.3
1	D	400	LEU	2.3
1	B	36	GLU	2.3
1	B	468	PRO	2.3
1	B	400	LEU	2.3
1	B	83	ASP	2.3
1	C	274	PHE	2.2
1	C	138	ILE	2.2
1	A	233	GLY	2.2
1	C	177	GLY	2.2
1	B	305	HIS	2.2
1	D	36	GLU	2.2
1	C	430	VAL	2.2
1	D	42	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	436	VAL	2.2
1	A	435	GLY	2.2
1	D	311	GLU	2.2
1	A	241	ALA	2.2
1	A	471	ALA	2.2
1	A	222	LYS	2.2
1	A	409	GLU	2.2
1	B	410	SER	2.2
1	A	40	GLY	2.2
1	D	484	HIS	2.2
1	D	325	LEU	2.2
1	B	39	GLU	2.2
1	D	354	PRO	2.2
1	B	47	GLN	2.2
1	C	222	LYS	2.1
1	D	79	LYS	2.1
1	B	432	ARG	2.1
1	C	192	PHE	2.1
1	B	42	ILE	2.1
1	D	474	LYS	2.1
1	C	300	GLY	2.1
1	D	322	TYR	2.1
1	B	277	ASP	2.1
1	B	220	GLN	2.1
1	A	477	HIS	2.1
1	B	222	LYS	2.1
1	D	137	ASN	2.1
1	C	54	GLY	2.1
1	C	157	LEU	2.1
1	D	369	CYS	2.1
1	A	37	ASP	2.1
1	D	407	ASP	2.1
1	D	246	TYR	2.1
1	A	82	GLY	2.1
1	B	332	GLY	2.1
1	B	133	ILE	2.1
1	D	170	LEU	2.1
1	B	440	ASP	2.1
1	C	196	GLN	2.1
1	B	321	CYS	2.1
1	D	34	TRP	2.1
1	A	86	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	319	SER	2.1
1	D	17	PRO	2.1
1	A	320	ILE	2.1
1	B	282	ILE	2.1
1	C	317	LEU	2.1
1	D	85	ARG	2.1
1	B	241	ALA	2.1
1	C	299	ALA	2.1
1	D	419	ALA	2.1
1	A	302	VAL	2.1
1	C	221	GLY	2.0
1	C	43	PRO	2.0
1	A	83	ASP	2.0
1	D	304	HIS	2.0
1	B	339	PHE	2.0
1	B	316	ILE	2.0
1	D	148	LEU	2.0
1	A	410	SER	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 carbohydrates 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	B-factors(Å^2)	Q<0.9
2	3ON	B	1491	32/32	0.45	0.56	62,84,99,100	0
2	3ON	D	1491	32/32	0.47	0.54	78,88,98,98	0
2	3ON	C	1491	32/32	0.49	0.53	75,89,103,104	0
2	3ON	A	1491	32/32	0.61	0.41	61,80,89,90	0
3	FE	D	1492	1/1	0.98	0.04	52,52,52,52	0

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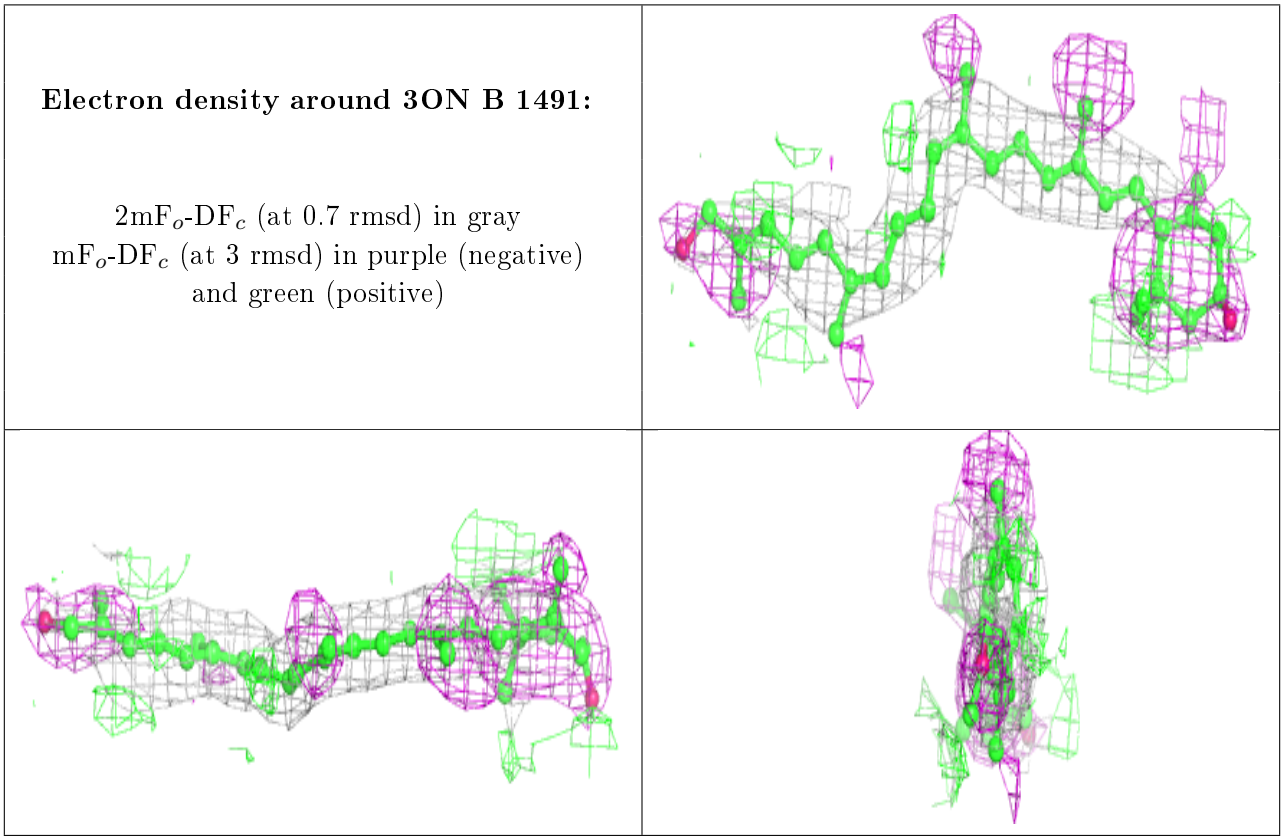
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FE	C	1492	1/1	0.99	0.03	51,51,51,51	0
3	FE	B	1492	1/1	0.99	0.04	45,45,45,45	0
3	FE	A	1492	1/1	1.00	0.02	43,43,43,43	0

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.

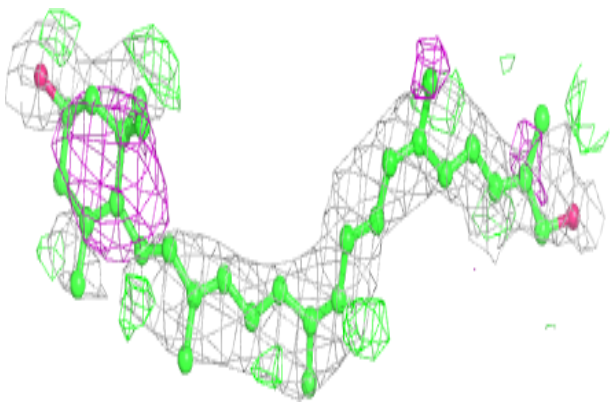
Electron density around 3ON B 1491:

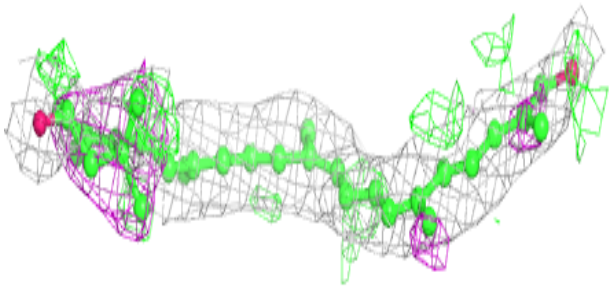
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

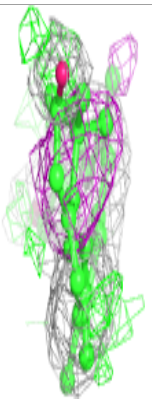


Electron density around 3ON D 1491:

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

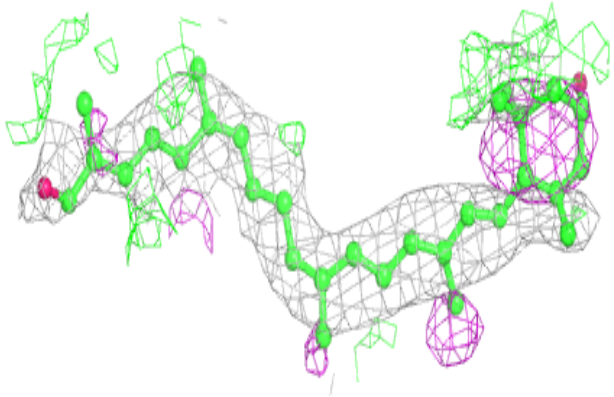


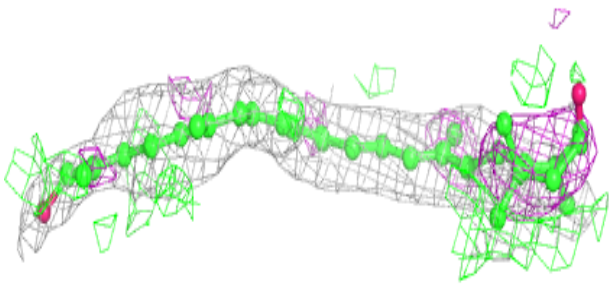


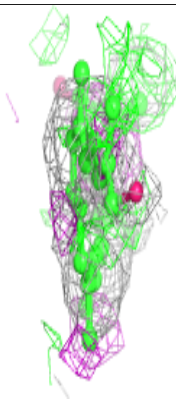


Electron density around 3ON C 1491:

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

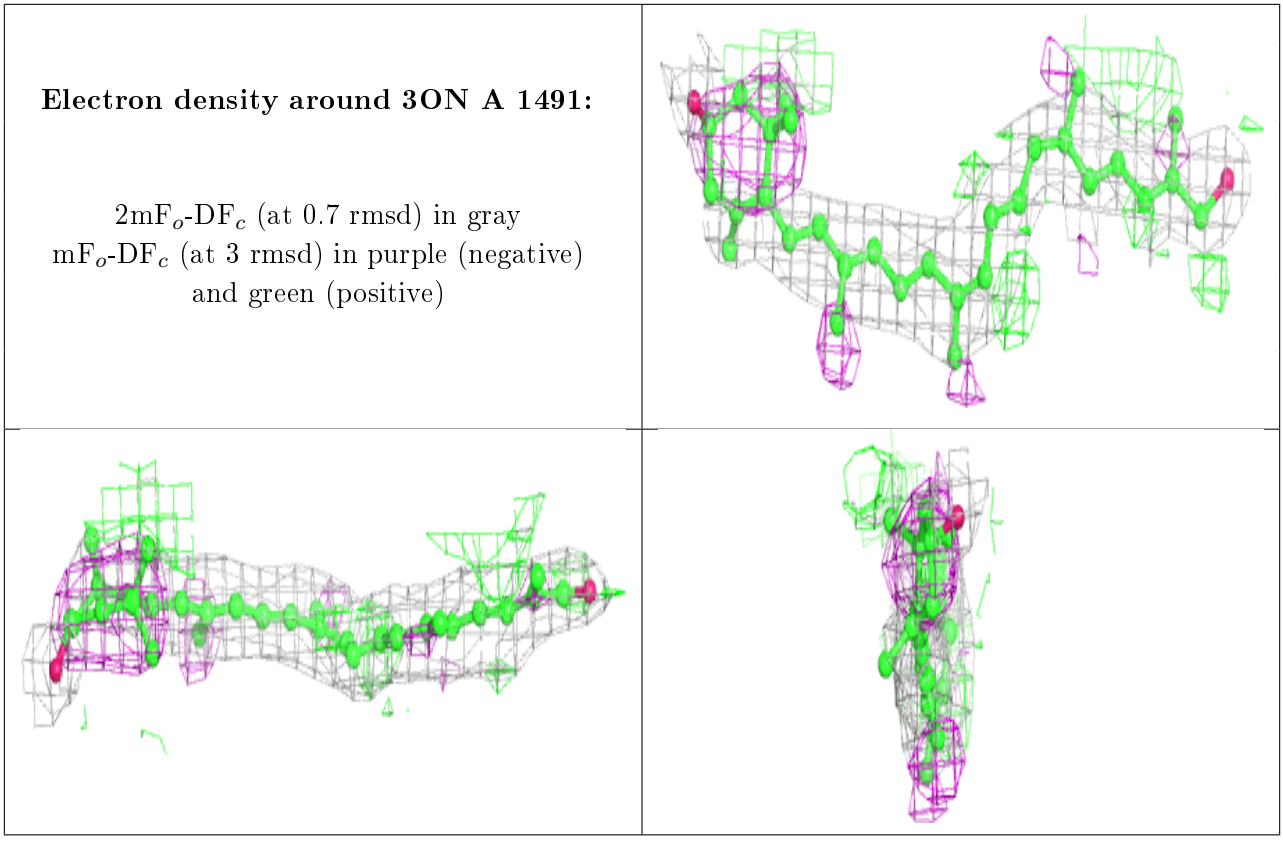






Electron density around 3ON A 1491:

$2mF_o$-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.