



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:11 PM UTC

PDB ID : 2BIW / pdb_00002biw
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

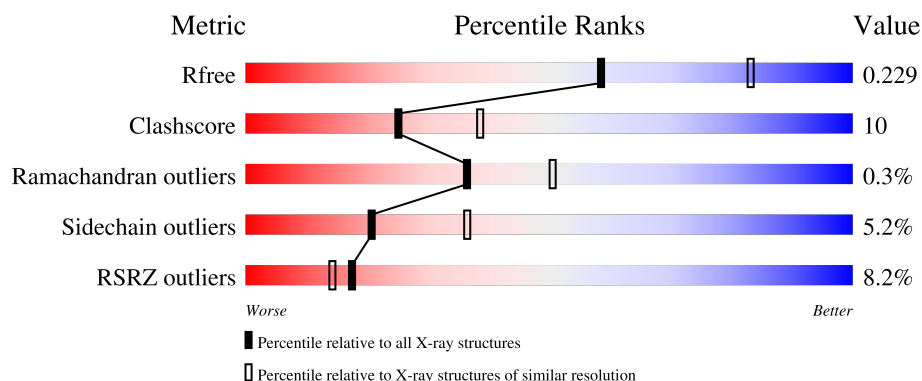
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	490	4% 76% 21% ..
1	B	490	7% 77% 19% ..
1	C	490	15% 78% 19% ..
1	D	490	6% 75% 21% ..

2 Entry composition [i](#)

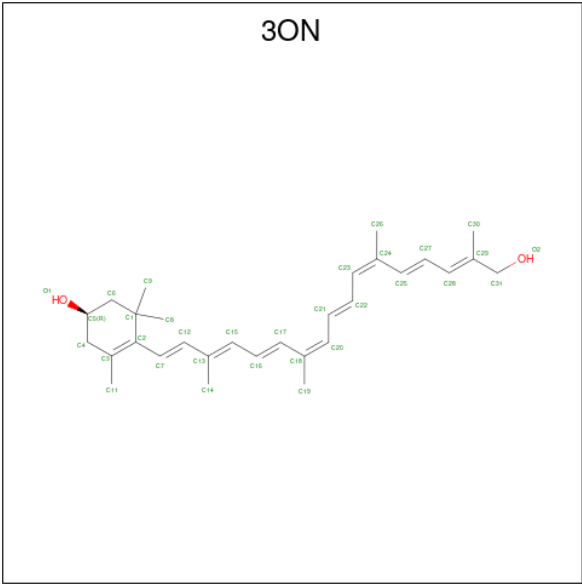
There are 4 unique types of molecules in this entry. The entry contains 15742 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 3ON) (formula: C₃₀H₄₂O₂).



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	0	0
			32	30	2		
2	D	1	Total	C	O	0	0
			32	30	2		

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

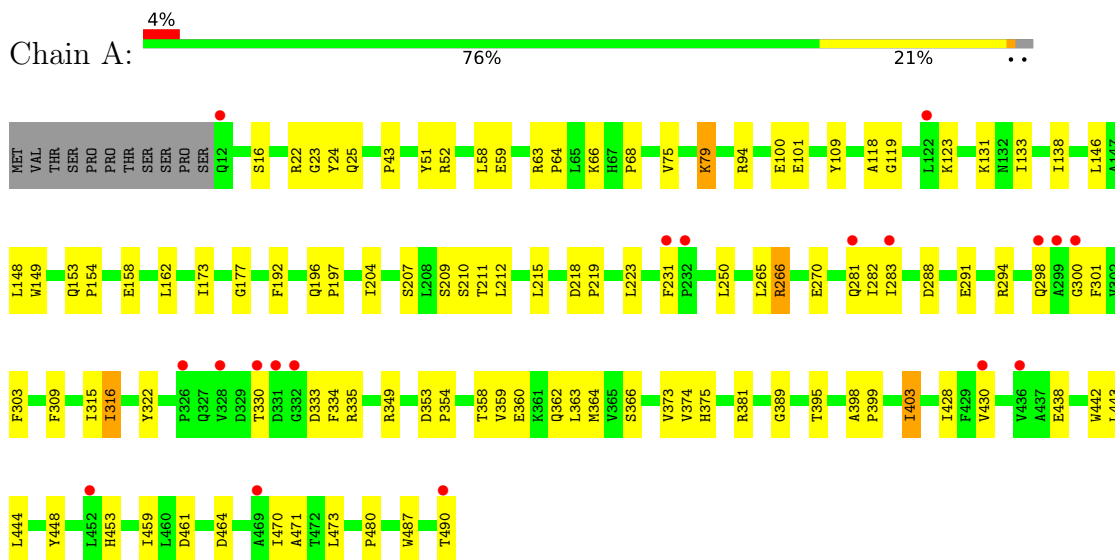
- Molecule 4 is water.

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

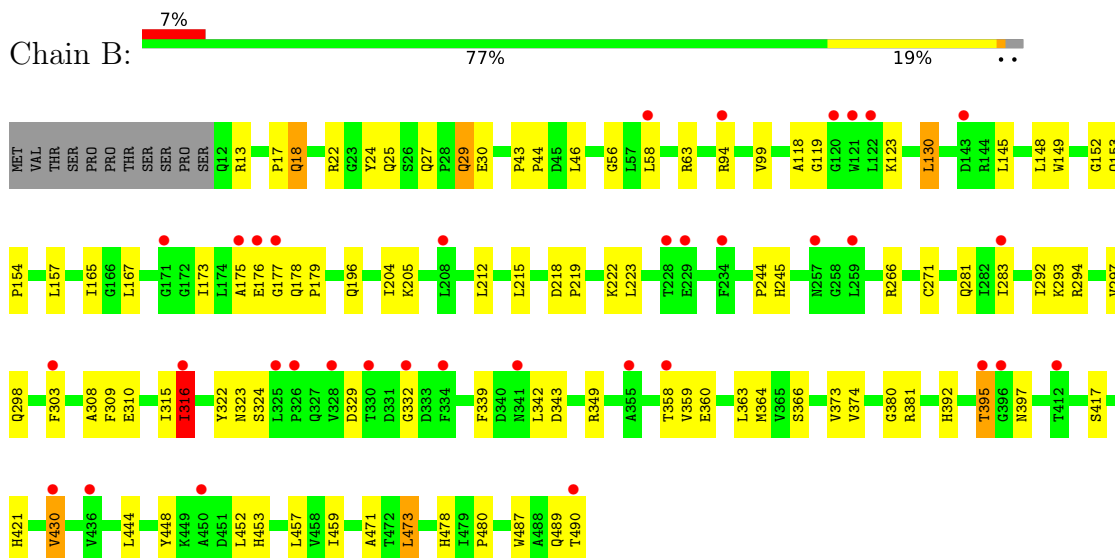
3 Residue-property plots

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.

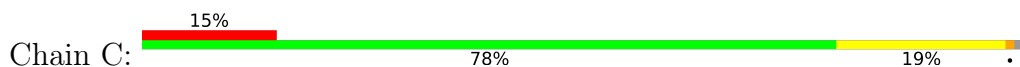
- Molecule 1: APOCAROTENOID-CLEAVING OXYGENASE

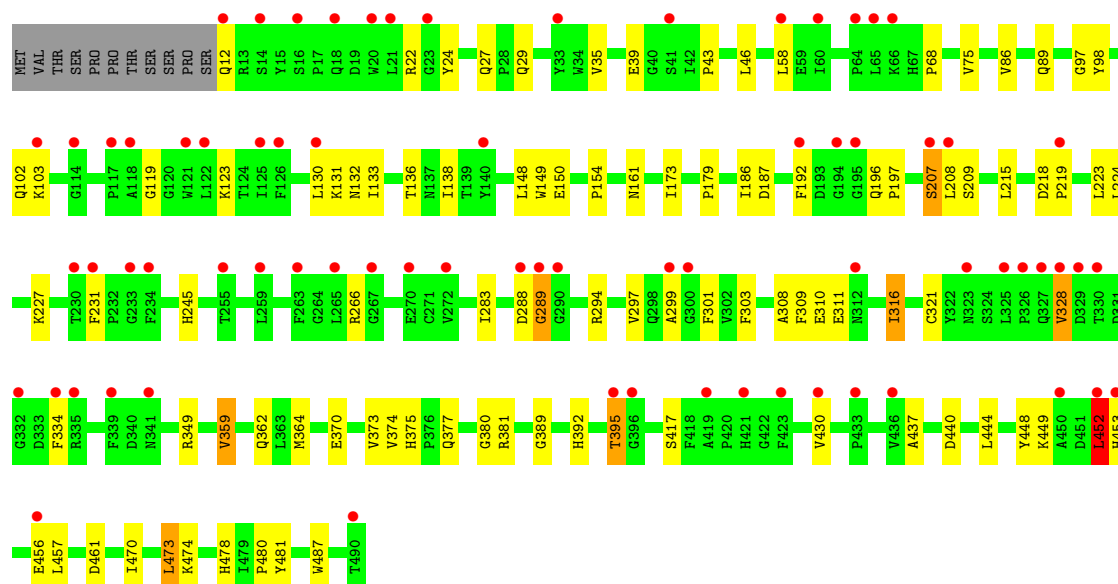


- Molecule 1: APOCAROTENOID-CLEAVING OXYGENASE

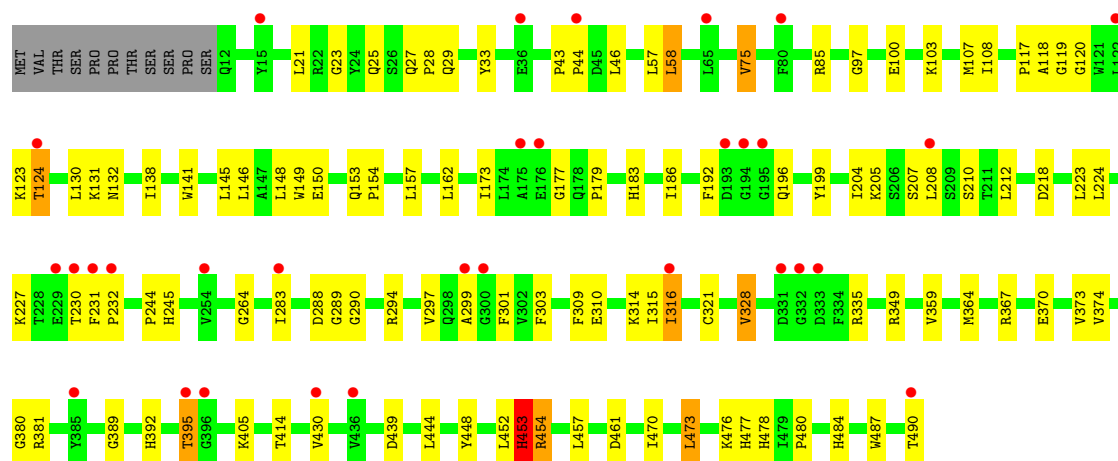
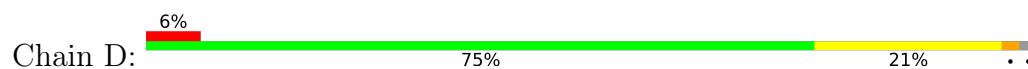


- Molecule 1: APOCAROTENOID-CLEAVING OXYGENASE





• Molecule 1: APOCAROTENOID-CLEAVING OXYGENASE



4 Data and refinement statistics

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 44.41 – 2.39	Depositor EDS
% Data completeness (in resolution range)	97.9 (44.41-2.39) 97.3 (44.41-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.35 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.047 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.86	1/3880 (0.0%)	0.97	6/5285 (0.1%)
1	B	0.88	1/3880 (0.0%)	0.95	5/5284 (0.1%)
1	C	0.80	1/3880 (0.0%)	0.94	8/5284 (0.2%)
1	D	0.78	2/3880 (0.1%)	0.95	14/5284 (0.3%)
All	All	0.83	5/15520 (0.0%)	0.95	33/21137 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	430	VAL	CA-CB	-6.79	1.47	1.53
1	D	85	ARG	NE-CZ	6.53	1.40	1.33
1	D	297	VAL	CA-CB	5.61	1.61	1.55
1	A	146	LEU	CA-C	-5.36	1.46	1.52
1	C	328	VAL	CA-CB	5.28	1.60	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	THR	CA-C-N	-9.42	111.43	122.83
1	A	395	THR	C-N-CA	-9.42	111.43	122.83
1	B	395	THR	N-CA-C	8.03	123.54	113.43
1	D	27	GLN	CA-C-N	7.55	127.19	119.19
1	D	27	GLN	C-N-CA	7.55	127.19	119.19
1	C	452	LEU	N-CA-C	-7.36	101.35	110.41
1	D	389	GLY	N-CA-C	-7.34	102.68	112.14
1	C	452	LEU	CA-C-N	-6.90	113.67	123.20
1	C	452	LEU	C-N-CA	-6.90	113.67	123.20
1	D	299	ALA	CA-C-N	-6.79	108.10	121.41
1	D	299	ALA	C-N-CA	-6.79	108.10	121.41
1	D	453	HIS	N-CA-C	-6.49	96.97	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	328	VAL	N-CA-CB	6.39	117.50	110.53
1	C	299	ALA	CA-C-N	-6.12	109.42	121.41
1	C	299	ALA	C-N-CA	-6.12	109.42	121.41
1	A	353	ASP	CA-C-N	6.03	125.74	119.05
1	A	353	ASP	C-N-CA	6.03	125.74	119.05
1	D	299	ALA	N-CA-C	5.86	120.98	113.18
1	B	430	VAL	CB-CA-C	-5.76	104.56	111.18
1	C	395	THR	CA-C-N	-5.74	110.72	123.12
1	C	395	THR	C-N-CA	-5.74	110.72	123.12
1	B	315	ILE	CA-C-N	-5.74	116.08	123.19
1	B	315	ILE	C-N-CA	-5.74	116.08	123.19
1	A	300	GLY	N-CA-C	-5.52	104.79	112.18
1	C	389	GLY	N-CA-C	-5.47	104.71	112.37
1	D	290	GLY	N-CA-C	-5.46	106.57	112.08
1	D	395	THR	CA-C-N	-5.43	110.77	121.41
1	D	395	THR	C-N-CA	-5.43	110.77	121.41
1	B	316	ILE	CB-CA-C	5.38	118.85	110.83
1	D	58	LEU	CA-CB-CG	-5.32	97.67	116.30
1	D	315	ILE	CA-C-N	-5.06	116.07	123.06
1	D	315	ILE	C-N-CA	-5.06	116.07	123.06
1	A	389	GLY	N-CA-C	-5.00	105.37	112.37

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	3767	0	3659	73	0
1	B	3767	0	3659	73	0
1	C	3767	0	3659	59	0
1	D	3767	0	3659	72	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	11	0
4	C	121	0	0	2	0
4	D	121	0	0	2	0
All	All	15742	0	14804	292	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 (292) 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
1:B:13:ARG:HH12	1:D:29:GLN:HE21	1.22	0.83
2:D:1491:3ON:H8C1	2:D:1491:3ON:H12	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:HH11	1:D:454:ARG:CG	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:HH11	1:D:454:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:B:316:ILE:C	1:B:316:ILE:HD12	2.26	0.61
2:B:1491:3ON:H9C1	2:B:1491:3ON:H12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:18:GLN:HE22	1:D:28:PRO:HB3	1.71	0.55
1:C:448:TYR:OH	1:C:453:HIS:CD2	2.54	0.55
1:B:18:GLN:H	1:B:18:GLN:HE21	1.54	0.55
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
1:A:153:GLN:HE21	1:A:177:GLY:H	1.54	0.54
2:A:1491:3ON:H6C1	4:A:2084:HOH:O	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:316:ILE:HD12	1:A:316:ILE:C	2.33	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
1:A:461:ASP:HB2	1:A:470:ILE:HD11	1.90	0.52
2:A:1491:3ON:H8C1	2:A:1491:3ON:C12	2.40	0.52
1:D:430:VAL:HG22	1:D:487:TRP:CD2	2.44	0.52
1:D:283:ILE:CD1	1:D:294:ARG:HE	2.23	0.51
1:D:303:PHE:CG	2:D:1491:3ON:C26	2.92	0.51
1:C:457:LEU:HD23	1:C:473:LEU:HD22	1.92	0.51
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:HA	1:A:291:GLU:OE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:17:PRO:HD2	1:D:28:PRO:HB2	1.96	0.48
1:C:196:GLN:HG3	1:C:197:PRO:HD2	1.94	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:C:480:PRO:O	1:C:481:TYR:C	2.58	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
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: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:43:PRO:HA	1:B:44:PRO:HD3	1.89	0.45
1:B:218:ASP:OD2	1:B:222:LYS:HB2	2.16	0.45
1:D:210:SER:HB2	1:D:231:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:265:LEU:C	1:A:266:ARG:HG2	2.41	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:35:VAL:HB	1:C:86:VAL:HG13	2.00	0.44
1:C:136:THR:OG1	2:C:1491:3ON:C19	2.66	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
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:A:250:LEU:C	1:A:250:LEU:HD23	2.44	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
1:D:43:PRO:HA	1:D:44:PRO:HD3	1.95	0.43
2:D:1491:3ON:H12	2:D:1491:3ON:C8	2.43	0.43
1:D:23:GLY:O	1:D:480:PRO:HA	2.17	0.43
1:D:124:THR:OG1	1:D:264:GLY:CA	2.67	0.43
1:A:63:ARG:HD2	1:A:118:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:79:LYS:HB2	1:A:79:LYS:HZ3	1.85	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:98:TYR:O	1:C:102:GLN:HG2	2.20	0.42
1:C:437:ALA:HB3	1:C:440:ASP:HB2	2.02	0.42
2:B:1491:3ON:H261	2:B:1491:3ON:H27	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
1:A:218:ASP:HB2	1:A:219:PRO:CD	2.51	0.41
2:A:1491:3ON:H16	2:A:1491:3ON:H141	1.92	0.41
1:B:177:GLY:C	4:B:2056:HOH:O	2.63	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
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:57:LEU:C	1:D:58:LEU:HG	2.45	0.41
1:D:97:GLY:HA3	1:D:131:LYS:HG3	2.03	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: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:148:LEU:HD23	1:B:154:PRO:HB3	2.02	0.41
1:B:323:ASN:ND2	4:B:2098:HOH:O	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:LYS:HA	1:C:123:LYS:HD3	1.90	0.41
1:D:309:PHE:CZ	1:D:316:ILE:CG1	3.02	0.41
1:D:477:HIS:HD2	1:D:478:HIS:O	2.04	0.41
1:A:101:GLU:OE1	1:A:131:LYS:NZ	2.50	0.41
2:A:1491:3ON:H261	2:A:1491:3ON:H27	1.36	0.41
1:B:152:GLY:C	1:B:179:PRO:HA	2.45	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:94:ARG:NH2	4:A:2037:HOH:O	2.53	0.40
1:A:298:GLN:HA	4:A:2102:HOH:O	2.21	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:A:464:ASP:OD1	1:A:464:ASP:C	2.65	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 ⓘ

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	477/490 (97%)	461 (97%)	15 (3%)	1 (0%)	43	58
1	B	477/490 (97%)	459 (96%)	17 (4%)	1 (0%)	43	58
1	C	477/490 (97%)	461 (97%)	14 (3%)	2 (0%)	30	43
1	D	477/490 (97%)	458 (96%)	17 (4%)	2 (0%)	30	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1908/1960 (97%)	1839 (96%)	63 (3%)	6 (0%)	36 50

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 ⓘ

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%)	22 38
1	B	399/410 (97%)	379 (95%)	20 (5%)	22 38
1	C	399/410 (97%)	379 (95%)	20 (5%)	22 38
1	D	399/410 (97%)	376 (94%)	23 (6%)	18 32
All	All	1596/1640 (97%)	1513 (95%)	83 (5%)	21 36

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	79	LYS
1	A	158	GLU
1	A	207	SER
1	A	209	SER
1	A	215	LEU
1	A	266	ARG
1	A	282	ILE
1	A	316	ILE

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Mol	Chain	Res	Type
1	A	358	THR
1	A	359	VAL
1	A	360	GLU
1	A	362	GLN
1	A	364	MET
1	A	373	VAL
1	A	374	VAL
1	A	381	ARG
1	A	403	ILE
1	A	473	LEU
1	A	490	THR
1	B	18	GLN
1	B	29	GLN
1	B	94	ARG
1	B	99	VAL
1	B	130	LEU
1	B	176	GLU
1	B	196	GLN
1	B	205	LYS
1	B	215	LEU
1	B	293	LYS
1	B	316	ILE
1	B	358	THR
1	B	364	MET
1	B	373	VAL
1	B	374	VAL
1	B	381	ARG
1	B	395	THR
1	B	452	LEU
1	B	473	LEU
1	B	490	THR
1	C	12	GLN
1	C	103	LYS
1	C	130	LEU
1	C	186	ILE
1	C	209	SER
1	C	215	LEU
1	C	231	PHE
1	C	266	ARG
1	C	311	GLU
1	C	316	ILE
1	C	328	VAL

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Mol	Chain	Res	Type
1	C	359	VAL
1	C	362	GLN
1	C	364	MET
1	C	373	VAL
1	C	374	VAL
1	C	395	THR
1	C	452	LEU
1	C	473	LEU
1	C	478	HIS
1	D	25	GLN
1	D	75	VAL
1	D	100	GLU
1	D	103	LYS
1	D	107	MET
1	D	124	THR
1	D	130	LEU
1	D	186	ILE
1	D	196	GLN
1	D	230	THR
1	D	314	LYS
1	D	316	ILE
1	D	328	VAL
1	D	359	VAL
1	D	364	MET
1	D	373	VAL
1	D	374	VAL
1	D	381	ARG
1	D	395	THR
1	D	414	THR
1	D	454	ARG
1	D	473	LEU
1	D	490	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	153	GLN
1	A	245	HIS
1	A	378	GLN
1	A	453	HIS
1	B	12	GLN

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Mol	Chain	Res	Type
1	B	18	GLN
1	B	27	GLN
1	B	153	GLN
1	B	226	GLN
1	B	245	HIS
1	B	253	ASN
1	B	298	GLN
1	B	323	ASN
1	B	362	GLN
1	B	378	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	102	GLN
1	C	153	GLN
1	C	155	HIS
1	C	196	GLN
1	C	245	HIS
1	C	298	GLN
1	C	323	ASN
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	253	ASN
1	D	312	ASN
1	D	378	GLN
1	D	393	HIS
1	D	397	ASN
1	D	453	HIS

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Mol	Chain	Res	Type
1	D	477	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	-	32,32,32	1.18	3 (9%)	40,42,42	2.77	18 (45%)
2	3ON	D	1491	-	32,32,32	1.33	4 (12%)	40,42,42	2.52	13 (32%)
2	3ON	B	1491	-	32,32,32	1.17	1 (3%)	40,42,42	3.03	18 (45%)
2	3ON	C	1491	-	32,32,32	1.25	2 (6%)	40,42,42	2.37	14 (35%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1491	3ON	C1-C2	3.54	1.58	1.53
2	C	1491	3ON	C6-C5	2.96	1.56	1.52
2	D	1491	3ON	C1-C2	2.93	1.57	1.53
2	A	1491	3ON	C6-C5	2.61	1.56	1.52
2	D	1491	3ON	C7-C2	2.54	1.53	1.45
2	A	1491	3ON	C1-C2	2.40	1.56	1.53
2	A	1491	3ON	C4-C5	2.11	1.55	1.52
2	D	1491	3ON	C4-C3	2.03	1.54	1.51
2	B	1491	3ON	C6-C5	2.02	1.55	1.52
2	D	1491	3ON	C3-C2	2.01	1.37	1.34

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1491	3ON	C25-C24-C23	6.61	129.41	119.01
2	D	1491	3ON	C25-C24-C23	6.59	129.37	119.01
2	D	1491	3ON	C26-C24-C25	-6.51	108.14	118.09
2	B	1491	3ON	C27-C28-C29	-6.47	118.59	127.69
2	B	1491	3ON	C25-C24-C23	6.34	128.98	119.01
2	B	1491	3ON	C1-C2-C3	-6.33	113.99	122.64
2	D	1491	3ON	C17-C18-C20	6.16	128.70	119.01
2	B	1491	3ON	C26-C24-C25	-6.15	108.69	118.09
2	C	1491	3ON	C17-C18-C20	6.04	128.51	119.01
2	A	1491	3ON	C22-C21-C20	-5.39	112.48	123.52
2	B	1491	3ON	C21-C22-C23	5.35	134.46	123.52
2	C	1491	3ON	C25-C24-C23	5.24	127.25	119.01
2	C	1491	3ON	C26-C24-C25	-5.22	110.11	118.09
2	C	1491	3ON	C1-C2-C3	-5.14	115.61	122.64
2	A	1491	3ON	C17-C18-C20	5.14	127.09	119.01
2	A	1491	3ON	C26-C24-C25	-5.07	110.35	118.09
2	A	1491	3ON	C1-C2-C3	-4.74	116.16	122.64
2	B	1491	3ON	C17-C18-C20	4.74	126.46	119.01
2	A	1491	3ON	C27-C28-C29	-4.68	121.11	127.69
2	B	1491	3ON	C22-C21-C20	-4.62	114.06	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1491	3ON	C21-C22-C23	4.53	132.80	123.52
2	C	1491	3ON	C1-C2-C7	4.29	127.28	115.65
2	B	1491	3ON	C11-C3-C2	-4.10	120.01	124.48
2	C	1491	3ON	C9-C1-C2	3.94	116.42	110.24
2	D	1491	3ON	C11-C3-C2	-3.86	120.27	124.48
2	D	1491	3ON	C9-C1-C2	3.84	116.27	110.24
2	C	1491	3ON	C19-C18-C20	-3.77	116.71	122.82
2	B	1491	3ON	C19-C18-C17	-3.77	112.33	118.09
2	A	1491	3ON	C1-C6-C5	3.75	121.81	113.59
2	B	1491	3ON	C27-C25-C24	-3.56	116.61	126.36
2	D	1491	3ON	C1-C2-C3	-3.49	117.87	122.64
2	A	1491	3ON	C1-C2-C7	3.47	125.06	115.65
2	A	1491	3ON	C11-C3-C2	-3.43	120.74	124.48
2	D	1491	3ON	C19-C18-C20	-3.41	117.29	122.82
2	D	1491	3ON	C1-C2-C7	3.39	124.83	115.65
2	B	1491	3ON	C1-C2-C7	3.38	124.83	115.65
2	B	1491	3ON	C11-C3-C4	3.33	120.55	114.42
2	A	1491	3ON	C27-C25-C24	-3.22	117.53	126.36
2	B	1491	3ON	C1-C6-C5	3.20	120.62	113.59
2	B	1491	3ON	C21-C20-C18	-3.11	122.91	127.28
2	A	1491	3ON	C11-C3-C4	3.06	120.06	114.42
2	D	1491	3ON	C27-C28-C29	2.91	131.78	127.69
2	B	1491	3ON	C14-C13-C15	-2.88	118.15	122.82
2	B	1491	3ON	C12-C13-C15	2.71	123.28	119.01
2	D	1491	3ON	C28-C27-C25	-2.71	115.35	123.20
2	D	1491	3ON	C19-C18-C17	-2.67	114.00	118.09
2	A	1491	3ON	C19-C18-C20	-2.62	118.58	122.82
2	A	1491	3ON	C19-C18-C17	-2.46	114.33	118.09
2	B	1491	3ON	C22-C23-C24	-2.40	123.92	127.28
2	D	1491	3ON	C31-C29-C28	-2.36	116.76	121.22
2	B	1491	3ON	C16-C15-C13	-2.35	123.98	127.28
2	C	1491	3ON	C11-C3-C4	2.35	118.75	114.42
2	C	1491	3ON	C22-C23-C24	-2.35	123.98	127.28
2	D	1491	3ON	C21-C22-C23	2.34	128.30	123.52
2	C	1491	3ON	C27-C25-C24	-2.25	120.18	126.36
2	A	1491	3ON	C21-C20-C18	-2.19	124.21	127.28
2	C	1491	3ON	C19-C18-C17	-2.17	114.77	118.09
2	C	1491	3ON	C15-C16-C17	-2.15	116.96	123.20
2	A	1491	3ON	C12-C13-C15	2.14	122.37	119.01
2	C	1491	3ON	C27-C28-C29	-2.09	124.76	127.69
2	A	1491	3ON	C26-C24-C23	-2.02	119.54	122.82
2	C	1491	3ON	C7-C2-C3	-2.00	116.95	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1491	3ON	C22-C23-C24	-2.00	124.47	127.28

There are no chirality outliers.

All (34) torsion outliers are listed below:

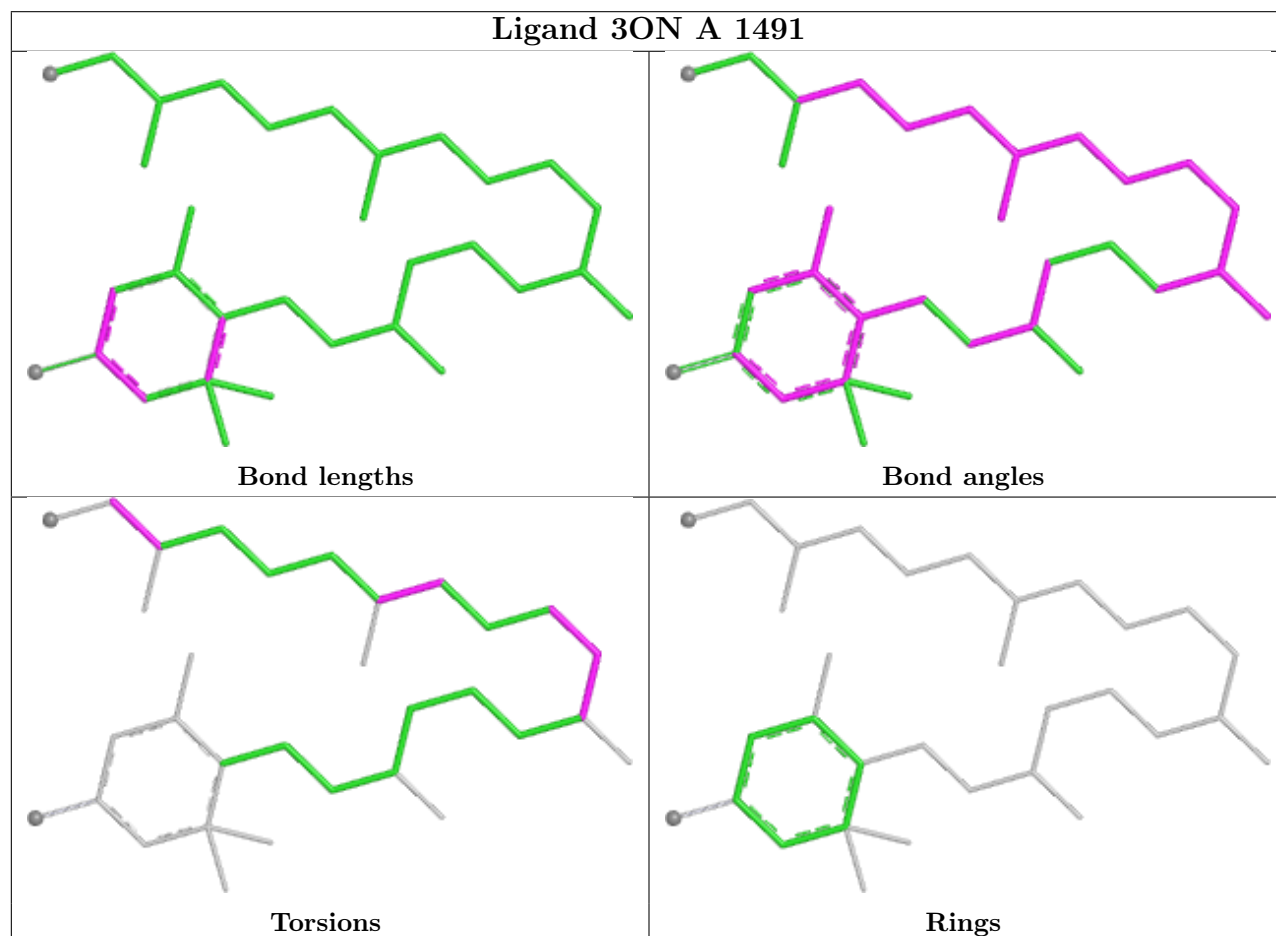
Mol	Chain	Res	Type	Atoms
2	D	1491	3ON	C7-C12-C13-C14
2	D	1491	3ON	C7-C12-C13-C15
2	B	1491	3ON	C22-C23-C24-C25
2	A	1491	3ON	C18-C20-C21-C22
2	B	1491	3ON	C18-C20-C21-C22
2	D	1491	3ON	C28-C29-C31-O2
2	A	1491	3ON	C22-C23-C24-C25
2	A	1491	3ON	C30-C29-C31-O2
2	B	1491	3ON	C30-C29-C31-O2
2	C	1491	3ON	C30-C29-C31-O2
2	D	1491	3ON	C30-C29-C31-O2
2	C	1491	3ON	C21-C22-C23-C24
2	A	1491	3ON	C28-C29-C31-O2
2	B	1491	3ON	C28-C29-C31-O2
2	A	1491	3ON	C19-C18-C20-C21
2	A	1491	3ON	C22-C23-C24-C26
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	D	1491	3ON	C19-C18-C20-C21
2	D	1491	3ON	C22-C23-C24-C26
2	A	1491	3ON	C17-C18-C20-C21
2	B	1491	3ON	C17-C18-C20-C21
2	C	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

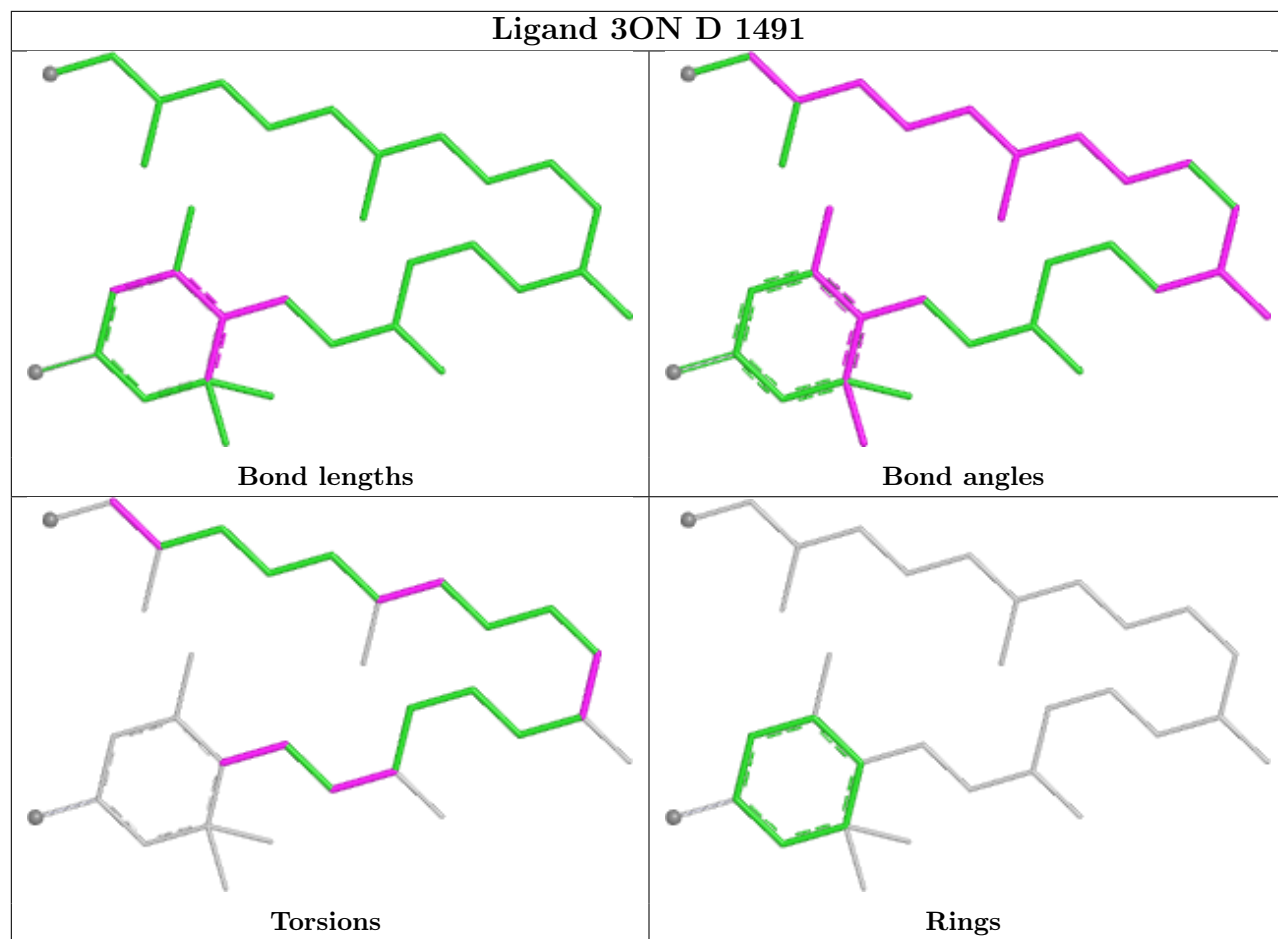
There are no ring outliers.

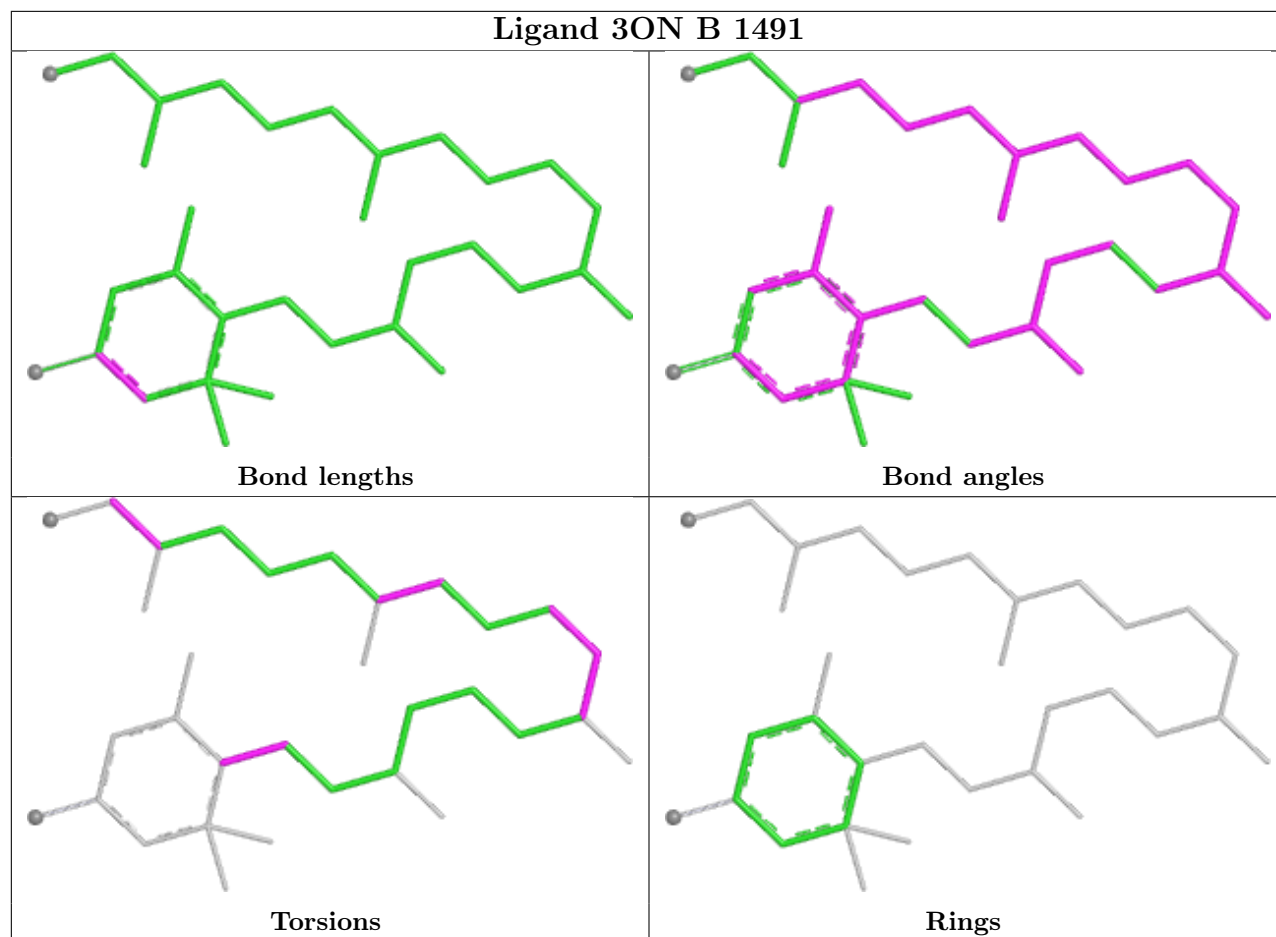
4 monomers are involved in 51 short contacts:

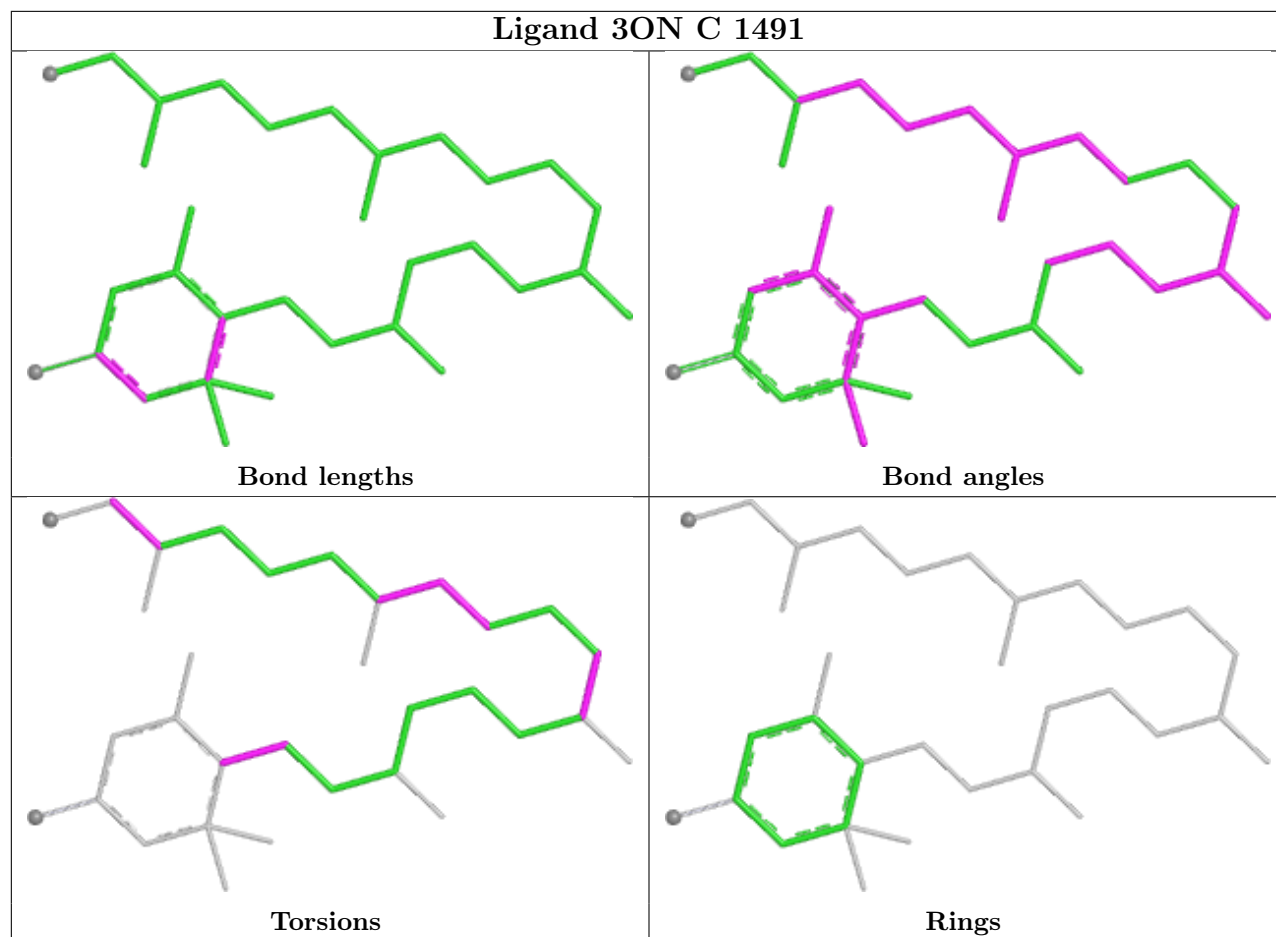
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1491	3ON	14	0
2	D	1491	3ON	12	0
2	B	1491	3ON	16	0
2	C	1491	3ON	9	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	479/490 (97%)	0.58	19 (3%) 42 38	55, 63, 74, 86	0
1	B	479/490 (97%)	0.76	35 (7%) 21 17	54, 63, 74, 86	0
1	C	479/490 (97%)	1.20	72 (15%) 5 4	56, 63, 74, 86	0
1	D	479/490 (97%)	0.86	31 (6%) 25 21	55, 63, 74, 87	0
All	All	1916/1960 (97%)	0.85	157 (8%) 17 14	54, 63, 74, 87	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	LEU	4.8
1	B	330	THR	4.5
1	A	331	ASP	4.4
1	C	332	GLY	4.1
1	D	231	PHE	4.1
1	C	122	LEU	4.0
1	D	299	ALA	3.8
1	B	430	VAL	3.8
1	B	177	GLY	3.8
1	C	208	LEU	3.7
1	C	121	TRP	3.6
1	B	328	VAL	3.6
1	D	232	PRO	3.6
1	C	452	LEU	3.6
1	D	395	THR	3.6
1	C	456	GLU	3.5
1	A	332	GLY	3.3
1	C	395	THR	3.3
1	A	430	VAL	3.3
1	C	64	PRO	3.3
1	C	192	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	58	LEU	3.2
1	C	230	THR	3.2
1	D	194	GLY	3.1
1	C	255	THR	3.1
1	C	263	PHE	3.1
1	A	328	VAL	3.1
1	B	412	THR	3.0
1	C	20	TRP	3.0
1	C	300	GLY	3.0
1	C	265	LEU	3.0
1	C	436	VAL	3.0
1	C	114	GLY	3.0
1	B	395	THR	3.0
1	C	233	GLY	3.0
1	A	299	ALA	2.9
1	D	208	LEU	2.9
1	C	231	PHE	2.9
1	A	12	GLN	2.9
1	C	23	GLY	2.9
1	C	125	ILE	2.9
1	C	396	GLY	2.8
1	D	254	VAL	2.8
1	D	430	VAL	2.8
1	C	207	SER	2.8
1	C	289	GLY	2.8
1	D	436	VAL	2.8
1	A	122	LEU	2.8
1	D	333	ASP	2.7
1	C	450	ALA	2.7
1	A	330	THR	2.7
1	D	331	ASP	2.7
1	C	290	GLY	2.7
1	D	300	GLY	2.7
1	D	229	GLU	2.7
1	A	452	LEU	2.7
1	B	436	VAL	2.7
1	C	328	VAL	2.7
1	A	490	THR	2.7
1	B	490	THR	2.7
1	C	103	LYS	2.7
1	C	234	PHE	2.6
1	B	332	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	332	GLY	2.6
1	C	130	LEU	2.6
1	B	334	PHE	2.6
1	B	341	ASN	2.6
1	D	193	ASP	2.6
1	B	120	GLY	2.6
1	B	228	THR	2.6
1	B	94	ARG	2.6
1	C	326	PRO	2.6
1	B	316	ILE	2.6
1	C	16	SER	2.6
1	C	325	LEU	2.5
1	C	194	GLY	2.5
1	B	303	PHE	2.5
1	C	12	GLN	2.5
1	B	176	GLU	2.5
1	C	299	ALA	2.5
1	C	60	ILE	2.4
1	A	469	ALA	2.4
1	B	175	ALA	2.4
1	C	117	PRO	2.4
1	B	121	TRP	2.4
1	C	329	ASP	2.4
1	D	44	PRO	2.4
1	C	330	THR	2.4
1	D	230	THR	2.4
1	B	325	LEU	2.4
1	A	436	VAL	2.3
1	A	281	GLN	2.3
1	C	21	LEU	2.3
1	C	327	GLN	2.3
1	C	312	ASN	2.3
1	B	171	GLY	2.3
1	D	490	THR	2.3
1	B	229	GLU	2.3
1	C	334	PHE	2.3
1	C	219	PRO	2.3
1	C	126	PHE	2.3
1	B	326	PRO	2.3
1	C	267	GLY	2.2
1	D	396	GLY	2.2
1	B	355	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	358	THR	2.2
1	A	283	ILE	2.2
1	B	283	ILE	2.2
1	C	272	VAL	2.2
1	B	257	ASN	2.2
1	A	232	PRO	2.2
1	C	433	PRO	2.2
1	C	18	GLN	2.2
1	D	316	ILE	2.2
1	B	234	PHE	2.2
1	C	323	ASN	2.2
1	A	300	GLY	2.2
1	B	396	GLY	2.2
1	D	195	GLY	2.2
1	C	339	PHE	2.2
1	C	341	ASN	2.2
1	B	208	LEU	2.1
1	C	65	LEU	2.1
1	A	231	PHE	2.1
1	C	270	GLU	2.1
1	D	176	GLU	2.1
1	D	124	THR	2.1
1	D	385	TYR	2.1
1	C	423	PHE	2.1
1	C	195	GLY	2.1
1	C	490	THR	2.1
1	C	66	LYS	2.1
1	C	33	TYR	2.1
1	C	288	ASP	2.1
1	D	283	ILE	2.1
1	A	326	PRO	2.1
1	C	41	SER	2.1
1	B	450	ALA	2.1
1	C	259	LEU	2.1
1	B	143	ASP	2.1
1	C	421	HIS	2.1
1	D	15	TYR	2.1
1	C	430	VAL	2.1
1	C	335	ARG	2.1
1	C	419	ALA	2.0
1	D	36	GLU	2.0
1	D	175	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	298	GLN	2.0
1	C	453	HIS	2.0
1	D	65	LEU	2.0
1	D	122	LEU	2.0
1	C	140	TYR	2.0
1	D	80	PHE	2.0
1	C	14	SER	2.0
1	C	118	ALA	2.0
1	B	259	LEU	2.0
1	C	58	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

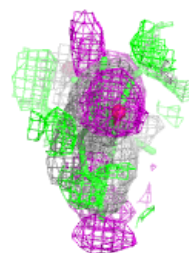
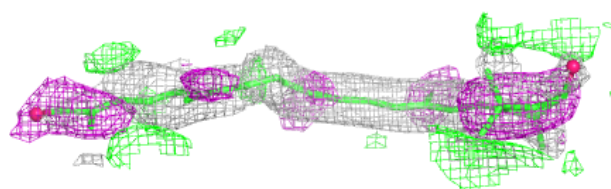
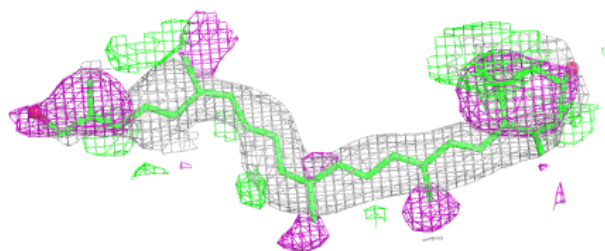
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	3ON	B	1491	32/32	0.71	0.32	62,84,99,100	0
2	3ON	C	1491	32/32	0.72	0.31	75,89,103,104	0
2	3ON	A	1491	32/32	0.75	0.28	61,80,89,90	0
2	3ON	D	1491	32/32	0.80	0.28	78,88,98,98	0
3	FE	C	1492	1/1	0.99	0.11	51,51,51,51	0
3	FE	D	1492	1/1	0.99	0.13	52,52,52,52	0
3	FE	A	1492	1/1	1.00	0.14	43,43,43,43	0
3	FE	B	1492	1/1	1.00	0.11	45,45,45,45	0

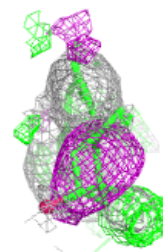
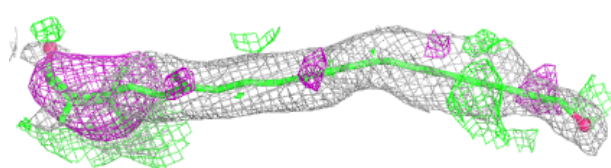
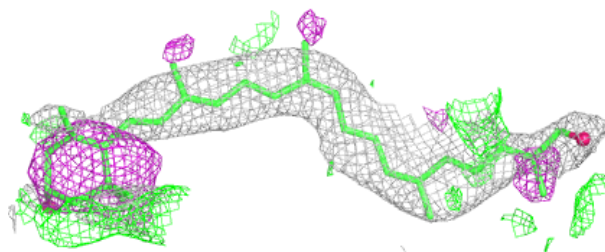
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

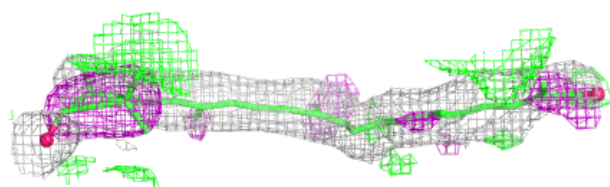
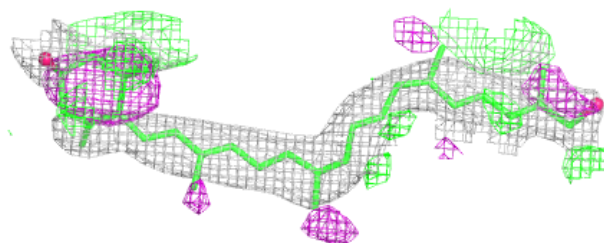
**Electron density around 3ON C 1491:**

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

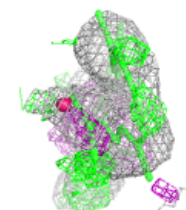
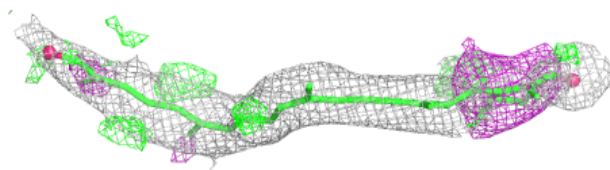
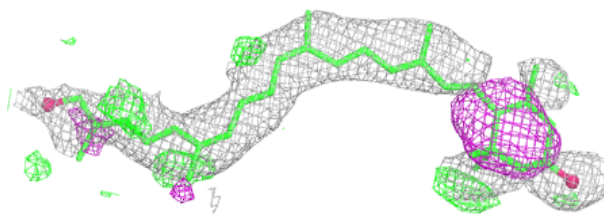


Electron density around 3ON A 1491:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.