



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2022 – 12:31 PM JST

PDB ID : 7FEA
Title : PY14 in complex with Col-D
Authors : Lin, C.C.; Ko, T.P.; Huang, K.F.; Yang, Y.L.
Deposited on : 2021-07-19
Resolution : 1.40 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 : 4.02b-467
Mogul : ?? (??), CSD ??CSD?? (????)
Xtriage (Phenix) : 1.13
EDS : 2.29
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) : 2.29

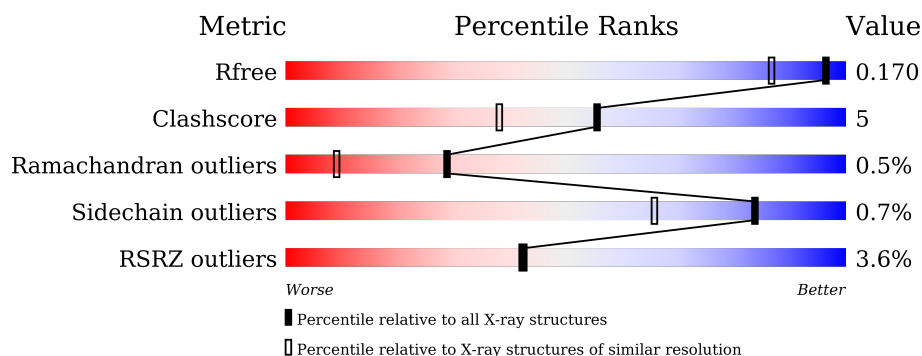
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	407	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	407	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>..</div> </div> </div>
1	C	407	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>.</div> </div> </div>
1	D	407	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>.</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13559 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 Acetyl-CoA C-acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	20	0
			2955	1843	543	557	12			
1	B	396	Total	C	N	O	S	0	15	0
			2948	1838	541	557	12			
1	C	396	Total	C	N	O	S	0	14	0
			2947	1842	539	554	12			
1	D	396	Total	C	N	O	S	0	17	0
			2958	1847	546	553	12			

There are 60 discrepancies between the modelled and reference sequences:

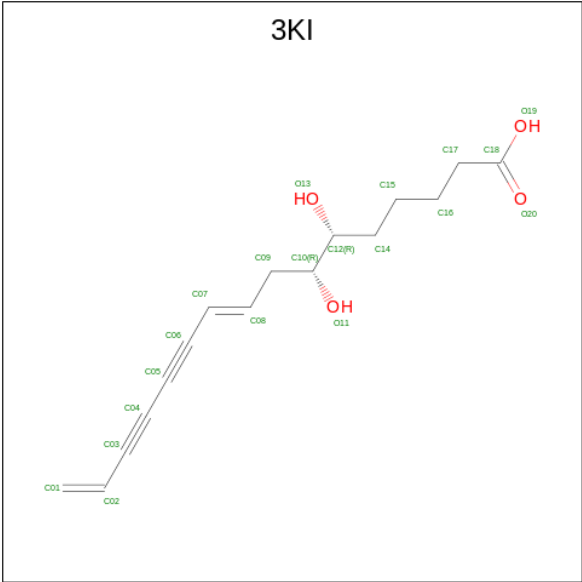
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A7U5Y2I6
A	2	VAL	-	expression tag	UNP A0A7U5Y2I6
A	395	LYS	-	expression tag	UNP A0A7U5Y2I6
A	396	LEU	-	expression tag	UNP A0A7U5Y2I6
A	397	ALA	-	expression tag	UNP A0A7U5Y2I6
A	398	ALA	-	expression tag	UNP A0A7U5Y2I6
A	399	ALA	-	expression tag	UNP A0A7U5Y2I6
A	400	LEU	-	expression tag	UNP A0A7U5Y2I6
A	401	GLU	-	expression tag	UNP A0A7U5Y2I6
A	402	HIS	-	expression tag	UNP A0A7U5Y2I6
A	403	HIS	-	expression tag	UNP A0A7U5Y2I6
A	404	HIS	-	expression tag	UNP A0A7U5Y2I6
A	405	HIS	-	expression tag	UNP A0A7U5Y2I6
A	406	HIS	-	expression tag	UNP A0A7U5Y2I6
A	407	HIS	-	expression tag	UNP A0A7U5Y2I6
B	1	MET	-	initiating methionine	UNP A0A7U5Y2I6
B	2	VAL	-	expression tag	UNP A0A7U5Y2I6
B	395	LYS	-	expression tag	UNP A0A7U5Y2I6
B	396	LEU	-	expression tag	UNP A0A7U5Y2I6
B	397	ALA	-	expression tag	UNP A0A7U5Y2I6
B	398	ALA	-	expression tag	UNP A0A7U5Y2I6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	399	ALA	-	expression tag	UNP A0A7U5Y2I6
B	400	LEU	-	expression tag	UNP A0A7U5Y2I6
B	401	GLU	-	expression tag	UNP A0A7U5Y2I6
B	402	HIS	-	expression tag	UNP A0A7U5Y2I6
B	403	HIS	-	expression tag	UNP A0A7U5Y2I6
B	404	HIS	-	expression tag	UNP A0A7U5Y2I6
B	405	HIS	-	expression tag	UNP A0A7U5Y2I6
B	406	HIS	-	expression tag	UNP A0A7U5Y2I6
B	407	HIS	-	expression tag	UNP A0A7U5Y2I6
C	1	MET	-	initiating methionine	UNP A0A7U5Y2I6
C	2	VAL	-	expression tag	UNP A0A7U5Y2I6
C	395	LYS	-	expression tag	UNP A0A7U5Y2I6
C	396	LEU	-	expression tag	UNP A0A7U5Y2I6
C	397	ALA	-	expression tag	UNP A0A7U5Y2I6
C	398	ALA	-	expression tag	UNP A0A7U5Y2I6
C	399	ALA	-	expression tag	UNP A0A7U5Y2I6
C	400	LEU	-	expression tag	UNP A0A7U5Y2I6
C	401	GLU	-	expression tag	UNP A0A7U5Y2I6
C	402	HIS	-	expression tag	UNP A0A7U5Y2I6
C	403	HIS	-	expression tag	UNP A0A7U5Y2I6
C	404	HIS	-	expression tag	UNP A0A7U5Y2I6
C	405	HIS	-	expression tag	UNP A0A7U5Y2I6
C	406	HIS	-	expression tag	UNP A0A7U5Y2I6
C	407	HIS	-	expression tag	UNP A0A7U5Y2I6
D	1	MET	-	initiating methionine	UNP A0A7U5Y2I6
D	2	VAL	-	expression tag	UNP A0A7U5Y2I6
D	395	LYS	-	expression tag	UNP A0A7U5Y2I6
D	396	LEU	-	expression tag	UNP A0A7U5Y2I6
D	397	ALA	-	expression tag	UNP A0A7U5Y2I6
D	398	ALA	-	expression tag	UNP A0A7U5Y2I6
D	399	ALA	-	expression tag	UNP A0A7U5Y2I6
D	400	LEU	-	expression tag	UNP A0A7U5Y2I6
D	401	GLU	-	expression tag	UNP A0A7U5Y2I6
D	402	HIS	-	expression tag	UNP A0A7U5Y2I6
D	403	HIS	-	expression tag	UNP A0A7U5Y2I6
D	404	HIS	-	expression tag	UNP A0A7U5Y2I6
D	405	HIS	-	expression tag	UNP A0A7U5Y2I6
D	406	HIS	-	expression tag	UNP A0A7U5Y2I6
D	407	HIS	-	expression tag	UNP A0A7U5Y2I6

- Molecule 2 is (6 {R},7 {R},9 {E})-6,7-bis(oxidanyl)hexadeca-9,15-dien-11,13-diynoic acid (three-letter code: 3KI) (formula: C₁₆H₂₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	16	4		
2	B	1	Total	C	O	0	0
			20	16	4		
2	C	1	Total	C	O	0	0
			20	16	4		
2	D	1	Total	C	O	0	0
			20	16	4		

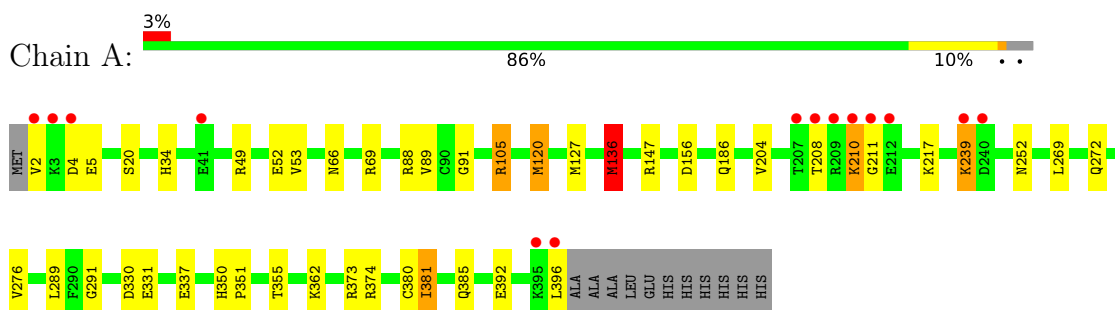
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	428	Total	O	0	0
			428	428		
3	B	414	Total	O	0	0
			414	414		
3	C	414	Total	O	0	0
			414	414		
3	D	415	Total	O	0	0
			415	415		

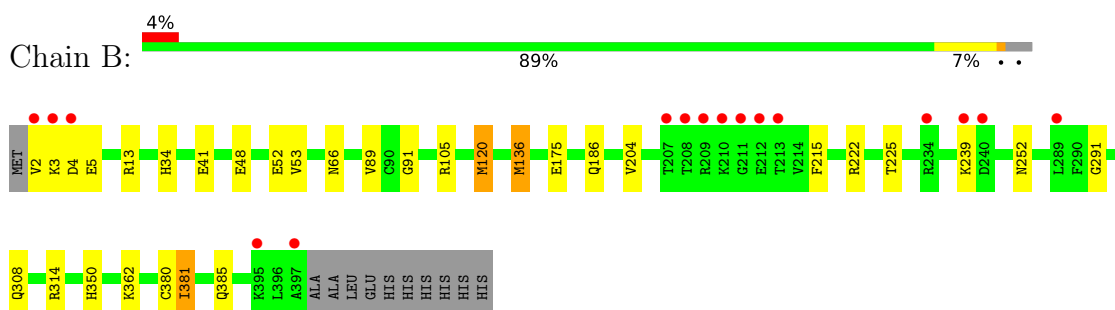
3 Residue-property plots [i](#)

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

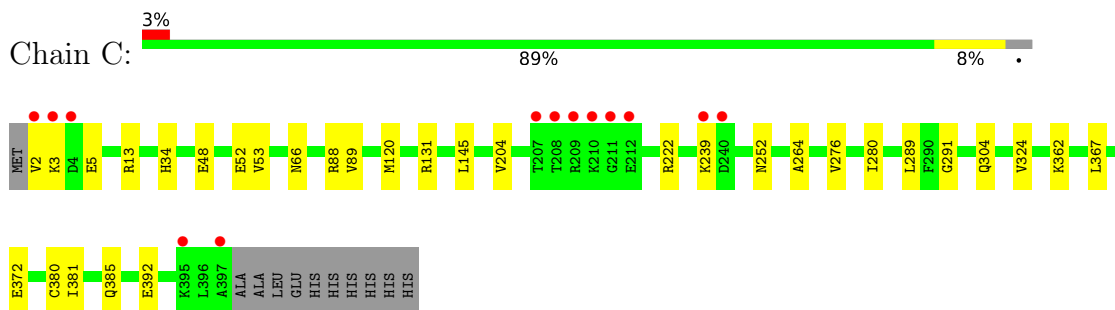
- Molecule 1: Acetyl-CoA C-acyltransferase



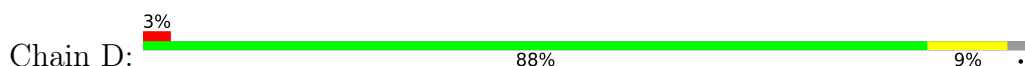
- Molecule 1: Acetyl-CoA C-acyltransferase

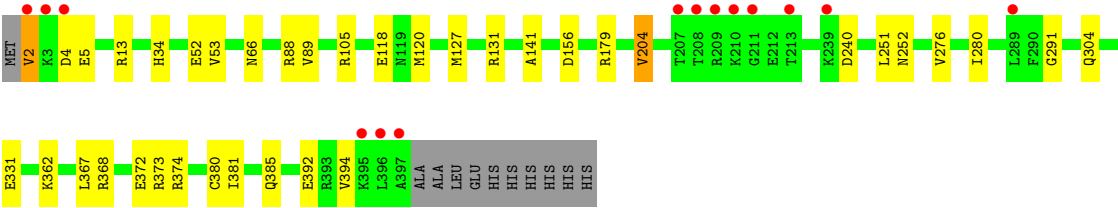


- Molecule 1: Acetyl-CoA C-acyltransferase



- Molecule 1: Acetyl-CoA C-acyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.94Å 77.74Å 98.12Å 70.76° 81.78° 65.00°	Depositor
Resolution (Å)	27.16 – 1.40 27.16 – 1.40	Depositor EDS
% Data completeness (in resolution range)	88.0 (27.16-1.40) 88.0 (27.16-1.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 1.40Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.146 , 0.163 0.146 , 0.170	Depositor DCC
R_{free} test set	1296 reflections (0.44%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13559	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.77	0/3097	0.95	11/4204 (0.3%)
1	B	0.74	4/3064 (0.1%)	0.89	8/4161 (0.2%)
1	C	0.70	0/3056	0.87	3/4151 (0.1%)
1	D	0.72	3/3081 (0.1%)	0.87	3/4183 (0.1%)
All	All	0.73	7/12298 (0.1%)	0.90	25/16699 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	175	GLU	CG-CD	7.56	1.63	1.51
1	B	308[A]	GLN	CG-CD	5.88	1.64	1.51
1	B	308[B]	GLN	CG-CD	5.88	1.64	1.51
1	D	118	GLU	CB-CG	5.56	1.62	1.52
1	B	175	GLU	CB-CG	5.36	1.62	1.52
1	D	204[A]	VAL	CB-CG1	-5.19	1.42	1.52
1	D	204[B]	VAL	CB-CG1	-5.19	1.42	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	13	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	A	381[A]	ILE	N-CA-C	-6.63	93.09	111.00
1	A	381[B]	ILE	N-CA-C	-6.63	93.09	111.00
1	A	136[A]	MET	CA-CB-CG	6.62	124.55	113.30
1	A	136[B]	MET	CA-CB-CG	6.62	124.55	113.30
1	B	381[A]	ILE	N-CA-C	-6.44	93.62	111.00
1	B	381[B]	ILE	N-CA-C	-6.44	93.62	111.00
1	A	147	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	13	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	D	13	ARG	NE-CZ-NH1	6.16	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	88	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	381[A]	ILE	CB-CA-C	-6.05	99.50	111.60
1	B	381[B]	ILE	CB-CA-C	-6.05	99.50	111.60
1	A	69	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	88	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	314	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	88	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	131	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	381[A]	ILE	CB-CA-C	-5.41	100.78	111.60
1	A	381[B]	ILE	CB-CA-C	-5.41	100.78	111.60
1	A	120[A]	MET	CA-CB-CG	-5.09	104.65	113.30
1	A	120[B]	MET	CA-CB-CG	-5.09	104.65	113.30
1	B	120[A]	MET	CA-CB-CG	-5.03	104.75	113.30
1	B	120[B]	MET	CA-CB-CG	-5.03	104.75	113.30
1	C	131	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2955	0	2988	45	1
1	B	2948	0	2965	26	0
1	C	2947	0	2992	23	0
1	D	2958	0	2998	32	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
2	C	20	0	0	1	0
2	D	20	0	0	0	0
3	A	428	0	0	15	2
3	B	414	0	0	11	3
3	C	414	0	0	6	0
3	D	415	0	0	15	2
All	All	13559	0	11943	123	4

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

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:HIS:ND1	1:A:355[B]:THR:HG21	1.86	0.91
1:A:105[A]:ARG:NH2	3:A:603:HOH:O	2.10	0.84
1:D:240[A]:ASP:OD2	3:D:601:HOH:O	1.95	0.82
1:A:136[A]:MET:SD	3:A:938:HOH:O	2.38	0.82
1:B:120[A]:MET:SD	3:B:603:HOH:O	2.38	0.81
1:D:5:GLU:OE1	3:D:602:HOH:O	1.98	0.80
1:C:239[B]:LYS:O	3:C:601:HOH:O	2.05	0.74
1:B:105:ARG:NH1	3:B:602:HOH:O	2.19	0.74
1:D:120[B]:MET:SD	3:D:607:HOH:O	2.46	0.73
1:C:34:HIS:CD2	1:C:204[A]:VAL:HG12	2.26	0.71
1:A:120[A]:MET:SD	3:A:605:HOH:O	2.49	0.71
1:B:3:LYS:HE3	1:B:4:ASP:OD2	1.93	0.69
1:D:381[B]:ILE:O	3:D:603:HOH:O	2.12	0.68
1:C:120[A]:MET:SD	3:C:602:HOH:O	2.51	0.68
1:D:34:HIS:CD2	1:D:204[B]:VAL:HG12	2.30	0.67
1:D:2:VAL:HA	1:D:5:GLU:HG3	1.78	0.65
1:D:4:ASP:HB2	3:D:611:HOH:O	1.97	0.64
1:A:291:GLY:HA2	1:A:380[B]:CYS:SG	2.36	0.64
1:A:351:PRO:HD2	1:A:355[B]:THR:HG22	1.79	0.64
1:A:380[A]:CYS:SG	3:A:851:HOH:O	2.55	0.64
1:A:4:ASP:O	1:A:105[A]:ARG:NH1	2.32	0.63
1:D:179[A]:ARG:NH2	3:D:604:HOH:O	2.12	0.62
1:C:291:GLY:HA2	1:C:380[B]:CYS:SG	2.39	0.62
1:A:381[A]:ILE:O	3:A:604:HOH:O	2.16	0.61
1:A:34:HIS:CD2	1:A:204[B]:VAL:HG22	2.36	0.61
1:C:280:ILE:H	1:C:304:GLN:NE2	1.99	0.61
1:D:373[A]:ARG:NE	1:D:392:GLU:OE2	2.29	0.60
1:D:2:VAL:HG22	1:D:5:GLU:OE2	2.02	0.59
1:B:291:GLY:HA2	1:B:380[B]:CYS:SG	2.42	0.59
1:D:291:GLY:HA2	1:D:380[B]:CYS:SG	2.42	0.59
1:A:34:HIS:CD2	1:A:204[A]:VAL:HG12	2.39	0.57
1:C:222:ARG:NH2	3:C:608:HOH:O	2.36	0.57
1:B:41[A]:GLU:HG3	3:B:740:HOH:O	2.03	0.57
1:B:3:LYS:HG3	1:B:4:ASP:N	2.20	0.57
1:D:2:VAL:N	3:D:611:HOH:O	2.39	0.55
1:D:331:GLU:OE1	3:D:605:HOH:O	2.18	0.54
1:B:186:GLN:HG3	3:B:604:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179[A]:ARG:HG3	3:D:831:HOH:O	2.08	0.54
1:B:34:HIS:CD2	1:B:204[A]:VAL:HG12	2.43	0.53
1:C:48:GLU:CD	1:C:48:GLU:H	2.12	0.53
1:B:2:VAL:HA	1:B:5:GLU:CD	2.28	0.52
1:A:362[B]:LYS:HE2	3:A:740:HOH:O	2.08	0.52
1:C:52:GLU:HG3	1:C:53:VAL:N	2.25	0.52
1:B:120[B]:MET:HG2	1:B:252:ASN:O	2.10	0.52
1:D:373[A]:ARG:HD3	1:D:374:ARG:NH1	2.24	0.52
1:A:351:PRO:O	1:A:355[B]:THR:HG23	2.10	0.52
1:B:136[A]:MET:HE2	1:D:251:LEU:HD11	1.91	0.52
1:A:276[B]:VAL:CG1	1:A:392:GLU:HB3	2.40	0.52
1:D:368:ARG:NH1	3:D:613:HOH:O	2.43	0.52
1:C:2:VAL:HA	1:C:5:GLU:HG3	1.92	0.52
1:D:280:ILE:H	1:D:304:GLN:NE2	2.09	0.51
1:B:136[A]:MET:HE1	3:D:623:HOH:O	2.11	0.51
1:B:350:HIS:O	3:B:603:HOH:O	2.20	0.50
1:A:272:GLN:HE22	1:A:396:LEU:CD2	2.25	0.50
1:A:362[B]:LYS:HG2	3:A:696:HOH:O	2.12	0.50
1:B:105:ARG:HD3	3:B:611:HOH:O	2.10	0.49
1:B:204[A]:VAL:HG23	1:B:215:PHE:HB3	1.94	0.49
1:B:381[A]:ILE:O	3:B:601:HOH:O	2.17	0.49
1:D:4:ASP:O	1:D:105:ARG:NH1	2.45	0.49
1:D:127[B]:MET:SD	1:D:141:ALA:HB2	2.53	0.49
1:D:120[A]:MET:HG2	1:D:252:ASN:O	2.13	0.49
1:A:331[B]:GLU:HG2	3:A:854:HOH:O	2.12	0.48
1:A:2:VAL:HG13	1:A:5:GLU:OE1	2.13	0.48
1:A:136[A]:MET:HE2	1:C:145:LEU:HD11	1.94	0.48
1:A:186[B]:GLN:HG2	3:A:904:HOH:O	2.14	0.48
1:B:222:ARG:NH2	3:B:613:HOH:O	2.40	0.47
1:D:362[B]:LYS:HG2	3:D:689:HOH:O	2.15	0.47
1:A:136[A]:MET:CE	1:C:145:LEU:HD11	2.44	0.47
1:C:276[B]:VAL:CG1	1:C:392:GLU:HB3	2.45	0.47
1:A:136[A]:MET:HE3	3:C:614:HOH:O	2.13	0.46
1:D:362[A]:LYS:HE3	3:D:704:HOH:O	2.15	0.46
1:A:291:GLY:N	3:A:606:HOH:O	2.27	0.46
1:B:52:GLU:HG3	1:B:53:VAL:N	2.30	0.46
1:A:208:THR:HG23	1:A:211:GLY:H	1.79	0.46
1:A:156:ASP:HB3	3:A:874:HOH:O	2.15	0.46
1:C:381:ILE:O	2:C:501:3KI:C01	2.64	0.46
1:C:291:GLY:N	3:C:605:HOH:O	2.35	0.46
1:B:48:GLU:H	1:B:48:GLU:CD	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362[A]:LYS:HE3	3:A:740:HOH:O	2.16	0.45
1:D:52:GLU:HG3	1:D:53:VAL:N	2.31	0.45
1:B:225:THR:O	3:B:604:HOH:O	2.20	0.45
1:C:362[B]:LYS:HG2	3:C:653:HOH:O	2.15	0.45
1:A:272:GLN:NE2	1:A:396:LEU:HD23	2.31	0.45
1:A:337[B]:GLU:HG3	3:A:945:HOH:O	2.16	0.45
1:C:3:LYS:HB2	1:C:264:ALA:HB2	1.99	0.45
1:A:52:GLU:HG3	1:A:53:VAL:N	2.32	0.45
1:A:276[B]:VAL:HG12	1:A:392:GLU:HB3	1.99	0.45
1:B:3:LYS:HE3	1:B:4:ASP:CG	2.36	0.45
1:A:373:ARG:HD3	1:A:374:ARG:NH1	2.32	0.44
1:A:210:LYS:HA	1:A:210:LYS:HD2	1.58	0.44
1:A:272:GLN:HE22	1:A:396:LEU:HD22	1.83	0.43
1:C:276[B]:VAL:HG12	1:C:392:GLU:HB3	2.01	0.43
1:B:204[A]:VAL:CG2	1:B:215:PHE:HB3	2.48	0.43
1:A:217:LYS:NZ	3:A:615:HOH:O	2.52	0.43
1:D:276[A]:VAL:HG23	1:D:394:VAL:HG22	2.01	0.42
1:A:2:VAL:HG13	1:A:5:GLU:CD	2.40	0.42
1:C:324:VAL:HG11	1:C:380[B]:CYS:SG	2.60	0.42
1:D:156[B]:ASP:OD1	3:D:606:HOH:O	2.22	0.42
1:D:276[A]:VAL:CG2	1:D:394:VAL:HG22	2.50	0.42
1:B:362:LYS:HE3	3:B:735:HOH:O	2.18	0.41
1:C:120[B]:MET:HG2	1:C:252:ASN:O	2.20	0.41
1:A:120[B]:MET:HG2	1:A:252:ASN:O	2.21	0.41
1:C:2:VAL:HG13	1:C:3:LYS:N	2.35	0.41
1:C:289:LEU:HA	1:C:289:LEU:HD23	1.80	0.41
1:D:367:LEU:HD22	1:D:372:GLU:HB2	2.02	0.41
1:C:367:LEU:HD22	1:C:372:GLU:HB2	2.03	0.41
1:D:276[B]:VAL:CG1	1:D:392:GLU:HB3	2.51	0.41
1:A:49:ARG:NH1	1:A:269:LEU:HD21	2.36	0.41
1:A:350:HIS:O	3:A:605:HOH:O	2.22	0.41
1:B:5:GLU:OE1	3:B:605:HOH:O	2.21	0.41
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.82	0.41
1:A:127[A]:MET:HE2	1:A:127[A]:MET:HB3	1.98	0.40
1:A:239[A]:LYS:HE2	1:A:239[A]:LYS:HB3	1.76	0.40
1:D:362[B]:LYS:HE2	3:D:704:HOH:O	2.21	0.40
1:A:2:VAL:HA	1:A:5:GLU:HG3	2.03	0.40
1:C:381:ILE:HB	1:C:385:GLN:HB2	2.04	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:962:HOH:O	3:D:932:HOH:O[1_546]	2.06	0.14
3:A:809:HOH:O	3:B:630:HOH:O[1_554]	2.07	0.13
3:A:944:HOH:O	3:B:943:HOH:O[1_554]	2.15	0.05
1:A:330:ASP:OD1	3:D:604:HOH:O[1_545]	2.17	0.03

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	413/407 (102%)	403 (98%)	8 (2%)	2 (0%)	29	9
1	B	409/407 (100%)	399 (98%)	8 (2%)	2 (0%)	29	9
1	C	408/407 (100%)	399 (98%)	7 (2%)	2 (0%)	29	9
1	D	411/407 (101%)	403 (98%)	6 (2%)	2 (0%)	29	9
All	All	1641/1628 (101%)	1604 (98%)	29 (2%)	8 (0%)	29	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	89	VAL
1	B	89	VAL
1	C	89	VAL
1	D	66	ASN
1	D	89	VAL
1	B	66	ASN
1	C	66	ASN

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	308/298 (103%)	299 (97%)	9 (3%)	42	11
1	B	303/298 (102%)	299 (99%)	4 (1%)	69	42
1	C	303/298 (102%)	303 (100%)	0	100	100
1	D	305/298 (102%)	304 (100%)	1 (0%)	92	81
All	All	1219/1192 (102%)	1205 (99%)	14 (1%)	84	50

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20[A]	SER
1	A	20[B]	SER
1	A	105[A]	ARG
1	A	105[B]	ARG
1	A	136[A]	MET
1	A	136[B]	MET
1	A	210	LYS
1	A	239[A]	LYS
1	A	239[B]	LYS
1	B	136[A]	MET
1	B	136[B]	MET
1	B	239[A]	LYS
1	B	239[B]	LYS
1	D	2	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	GLN
1	B	263	HIS
1	C	304	GLN
1	D	304	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

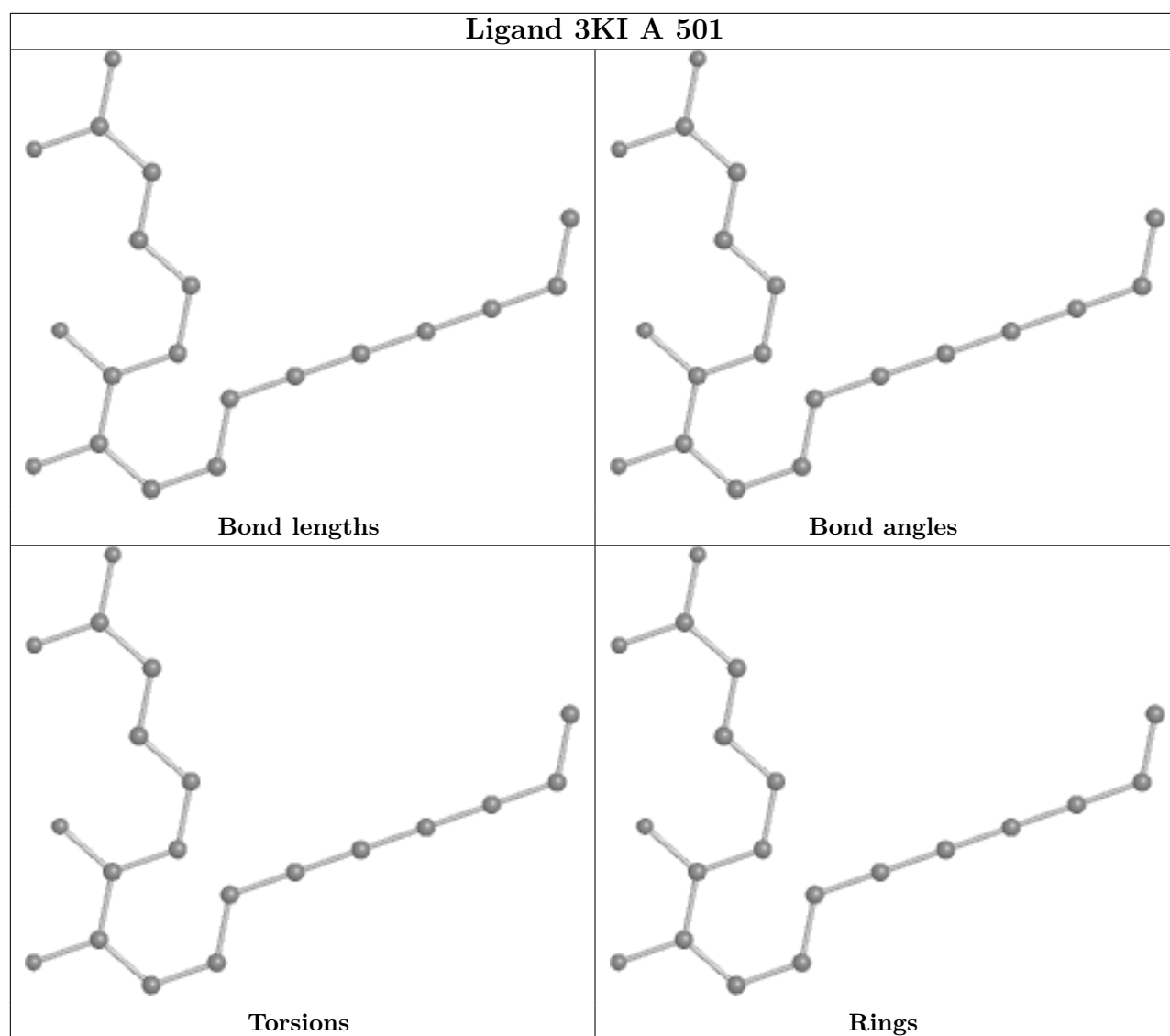
There are no chirality outliers.

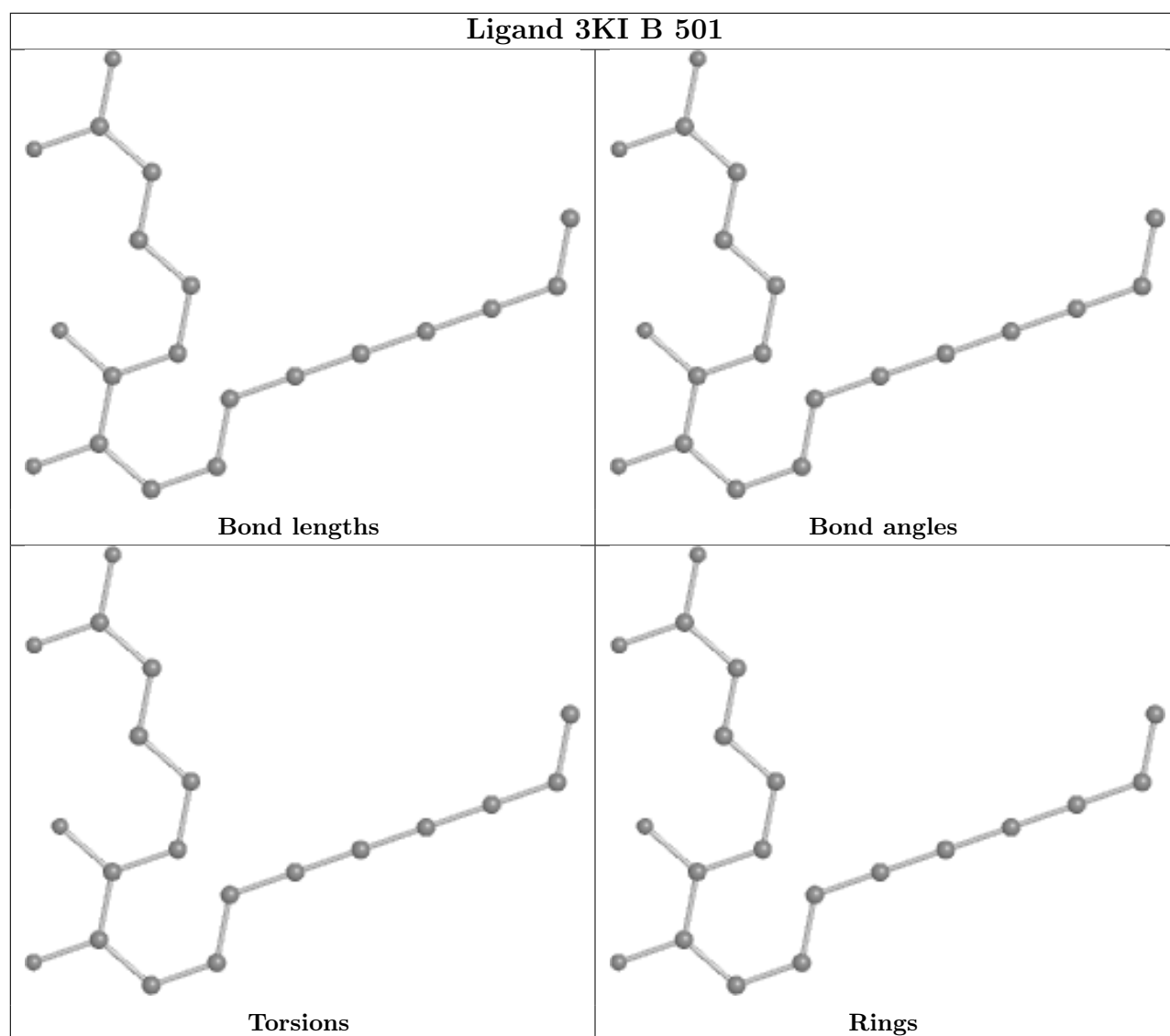
There are no torsion outliers.

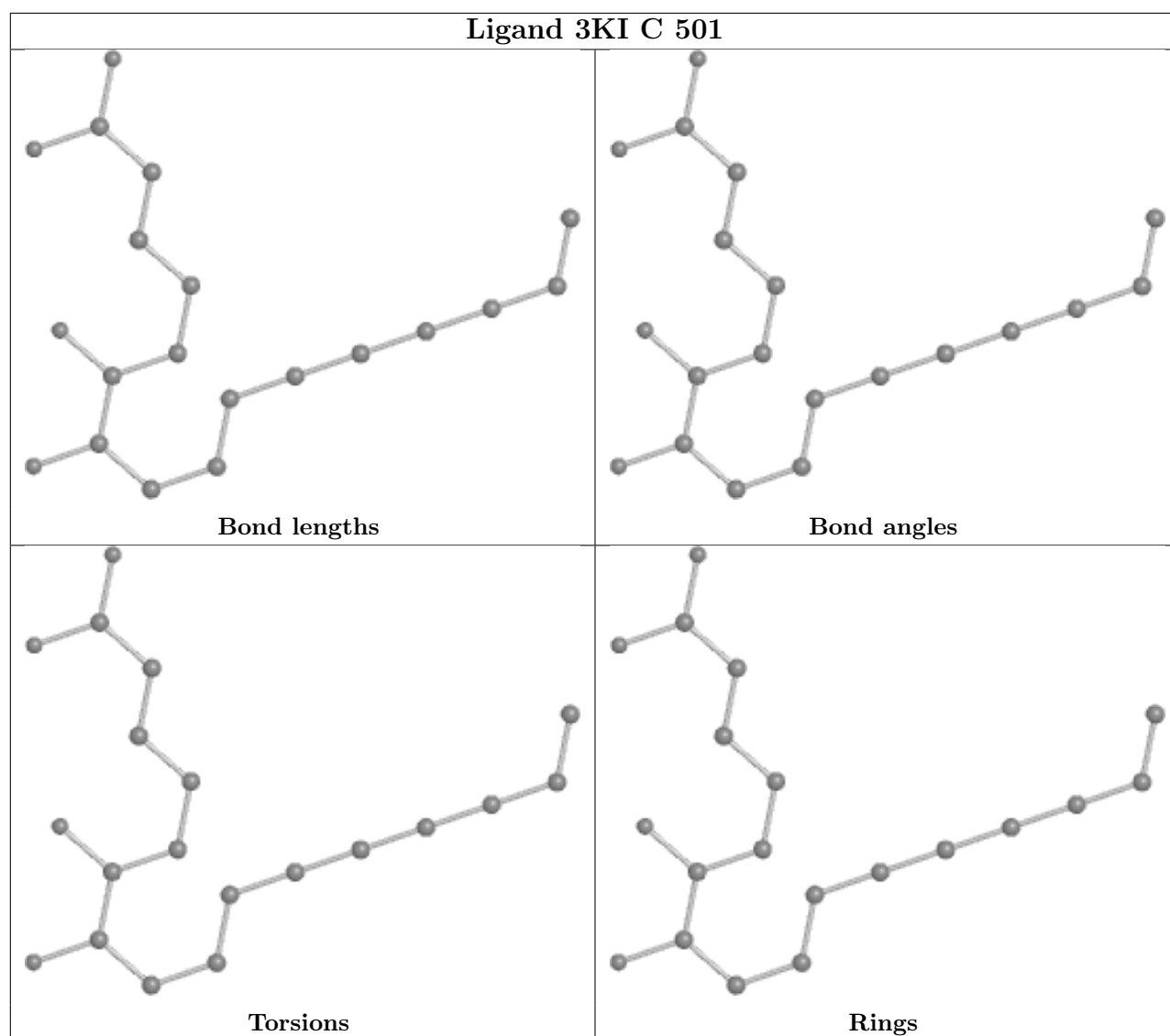
There are no ring outliers.

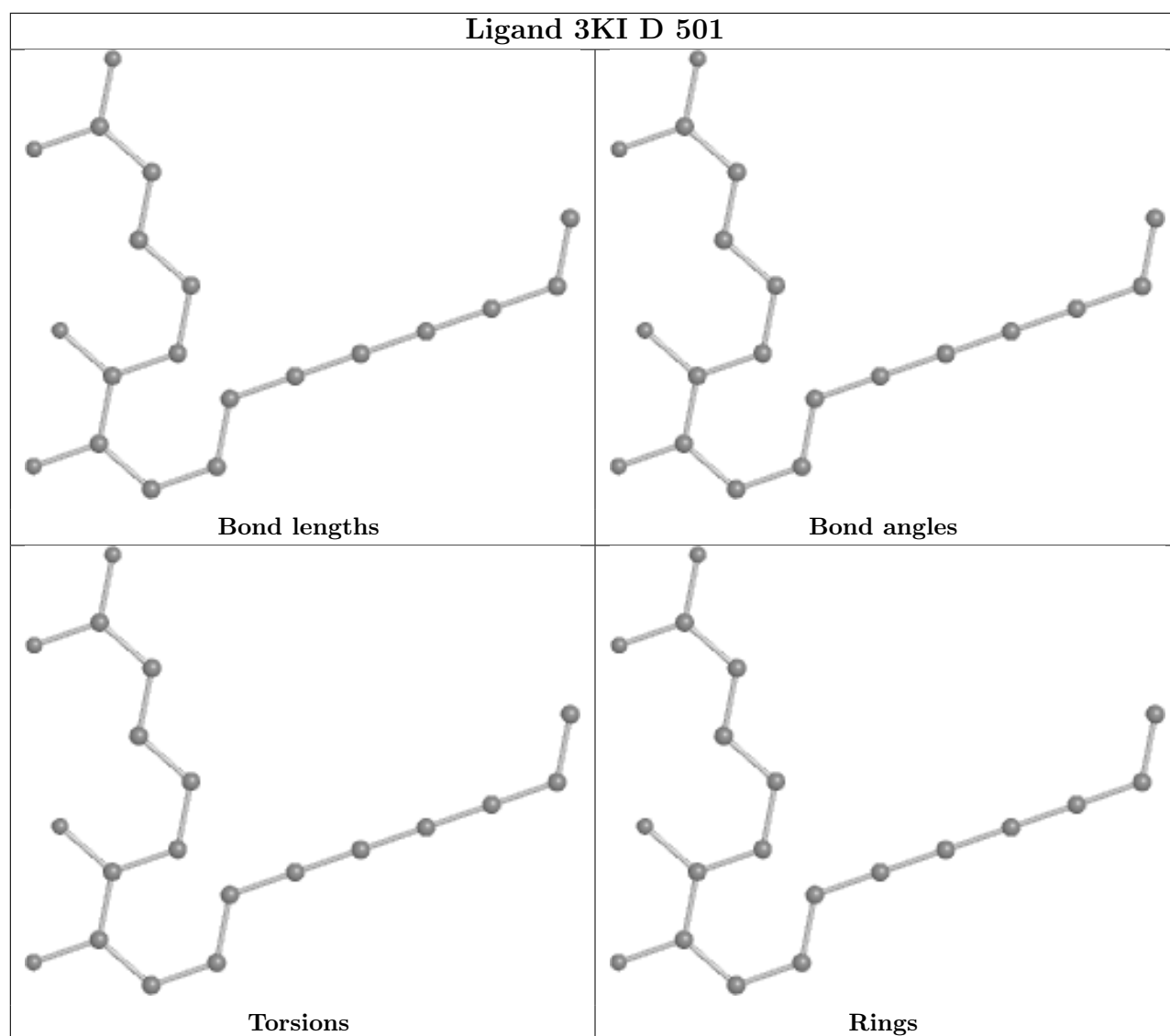
No monomer is involved in short contacts.

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	395/407 (97%)	-0.23	14 (3%) 44 43	9, 14, 34, 106	0
1	B	396/407 (97%)	-0.20	16 (4%) 38 39	9, 17, 38, 111	0
1	C	396/407 (97%)	-0.19	13 (3%) 46 46	10, 16, 37, 104	0
1	D	396/407 (97%)	-0.19	14 (3%) 44 43	9, 16, 38, 108	0
All	All	1583/1628 (97%)	-0.20	57 (3%) 42 42	9, 16, 38, 111	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	VAL	17.9
1	B	2	VAL	13.8
1	A	2	VAL	10.2
1	D	209	ARG	8.4
1	C	2	VAL	8.1
1	C	209	ARG	7.8
1	D	397	ALA	7.4
1	B	209	ARG	7.2
1	C	208	THR	7.0
1	D	210	LYS	7.0
1	A	209	ARG	7.0
1	D	208	THR	6.8
1	A	396	LEU	6.4
1	D	396	LEU	6.4
1	B	208	THR	6.3
1	A	210	LYS	6.3
1	B	210	LYS	6.2
1	A	208	THR	5.6
1	C	210	LYS	5.4
1	C	239[A]	LYS	4.8
1	D	3	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	211	GLY	4.4
1	A	3	LYS	4.2
1	C	3	LYS	4.0
1	C	397	ALA	3.9
1	B	211	GLY	3.9
1	B	240[A]	ASP	3.9
1	D	4	ASP	3.8
1	B	3	LYS	3.6
1	A	239[A]	LYS	3.6
1	B	397	ALA	3.5
1	A	207	THR	3.5
1	D	207	THR	3.5
1	B	239[A]	LYS	3.4
1	C	207	THR	3.3
1	A	395	LYS	3.3
1	D	239[A]	LYS	3.3
1	C	211	GLY	3.2
1	B	207	THR	3.0
1	C	240[A]	ASP	3.0
1	B	234	ARG	2.9
1	C	4	ASP	2.9
1	A	211	GLY	2.8
1	B	289	LEU	2.7
1	B	212	GLU	2.6
1	D	213	THR	2.6
1	B	213	THR	2.6
1	D	395	LYS	2.4
1	A	4	ASP	2.3
1	B	4	ASP	2.3
1	A	240[A]	ASP	2.2
1	A	212	GLU	2.1
1	C	395	LYS	2.1
1	C	212	GLU	2.1
1	D	289	LEU	2.0
1	A	41	GLU	2.0
1	B	395	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

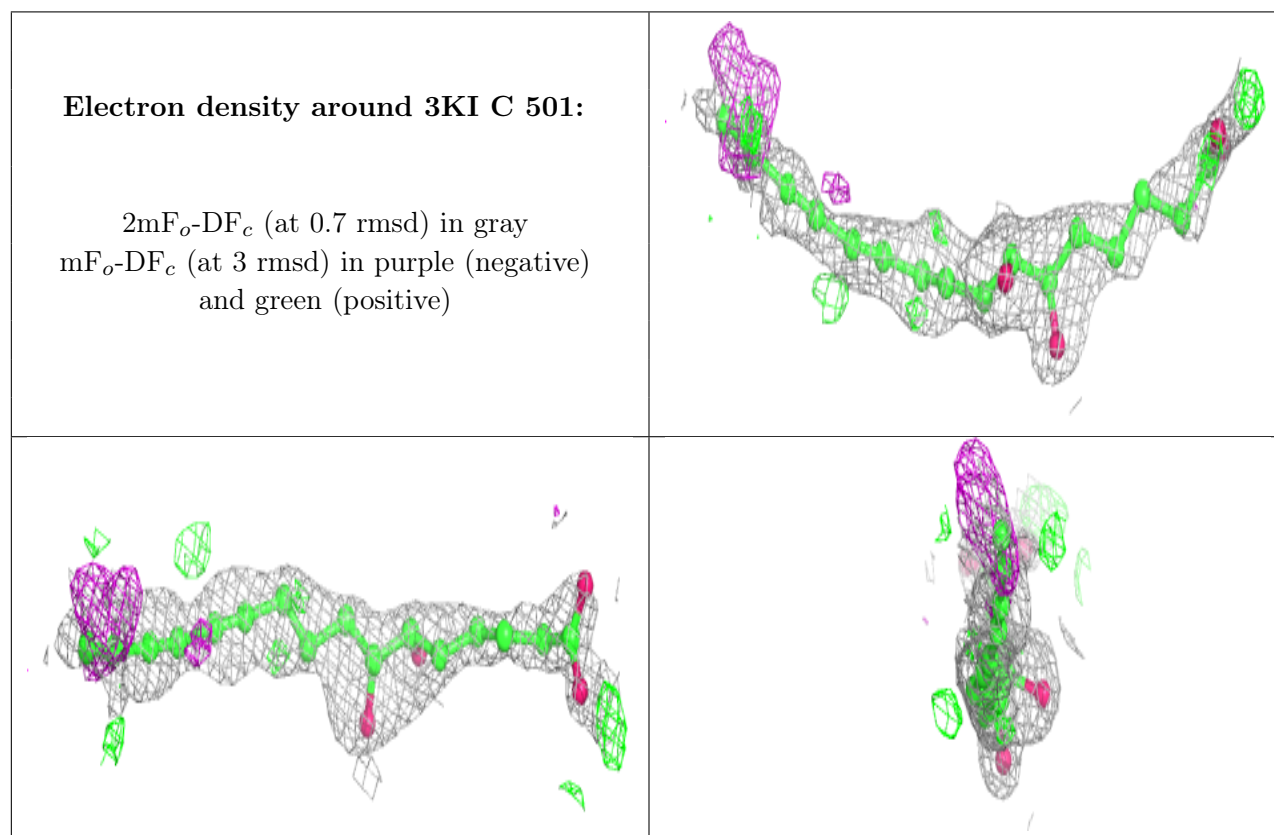
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

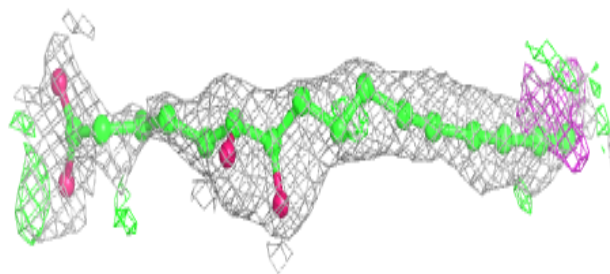
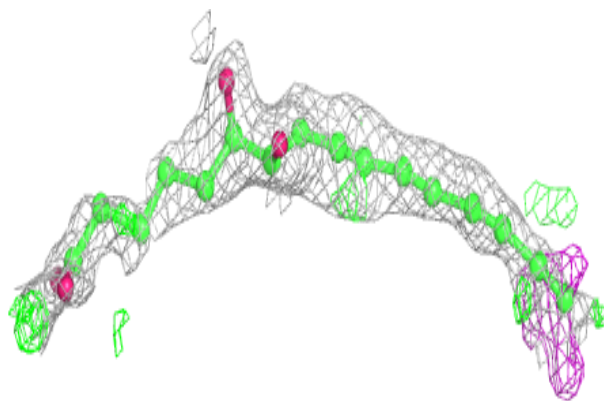
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	3KI	C	501	20/20	0.59	0.21	36,50,69,70	0
2	3KI	B	501	20/20	0.63	0.19	33,53,77,77	0
2	3KI	A	501	20/20	0.66	0.19	37,48,68,69	0
2	3KI	D	501	20/20	0.68	0.22	37,53,75,76	0

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.

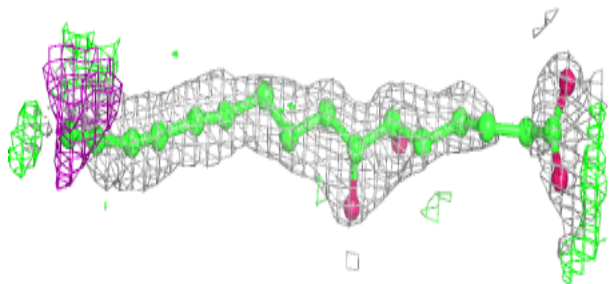
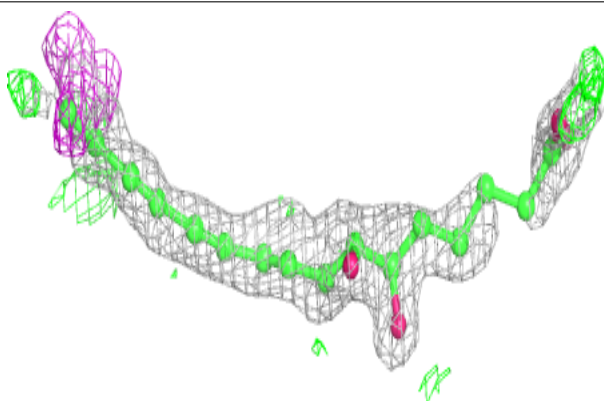


Electron density around 3KI B 501:

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

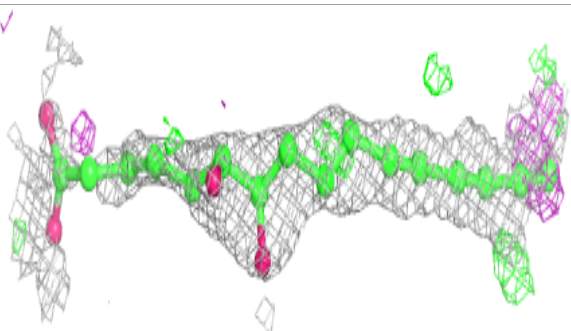
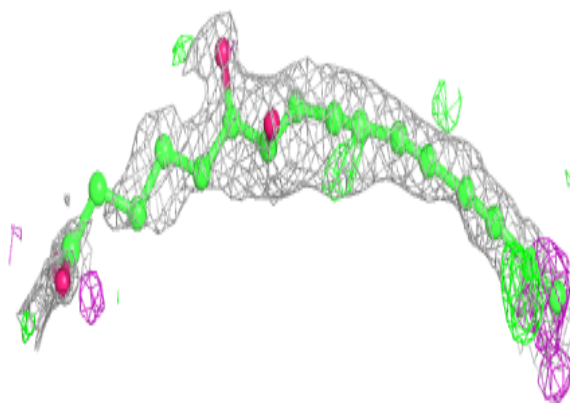
**Electron density around 3KI A 501:**

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



Electron density around 3KI D 501:

$2mF_o-DF_c$ (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.