WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2023 – 09:39 AM EST

PDB ID	:	5USR
Title	:	Crystal structure of human NFS1-ISD11 in complex with E. coli acyl-carrier protein at 3.09 angstroms
Authors	:	Cory, S.A.; Barondeau, D.P.
Deposited on	:	2017-02-13
Resolution	:	3.09 Å(reported)

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	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.09 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.
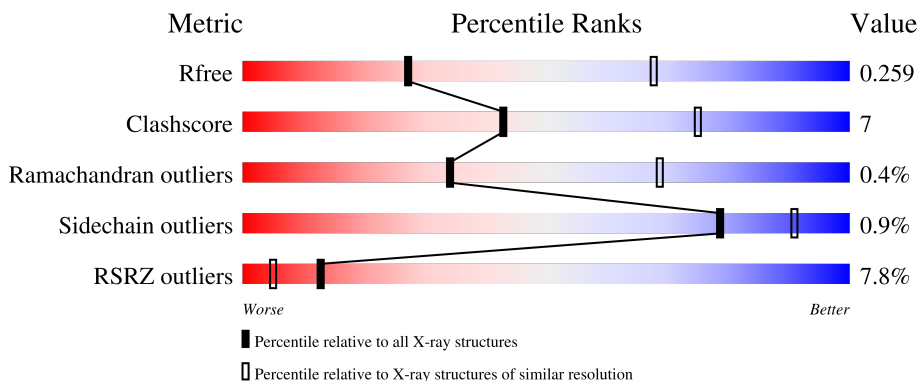
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	426	
1	C	426	
1	E	426	
1	G	426	
2	B	91	

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Mol	Chain	Length	Quality of chain
2	D	91	2% / 74% / 14% / 12%
2	F	91	3% / 74% / 9% / 18%
2	H	91	% / 73% / 12% / 15%
3	I	78	9% / 73% / 24% / .
3	J	78	38% / 86% / 10% / .
3	K	78	24% / 73% / 15% / 12%
3	L	78	33% / 72% / 19% / 9%

2   Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 15666 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 Cysteine desulfurase, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	P	S	0	0	0
			2877	1810	504	544	1	18			
1	C	352	Total	C	N	O	P	S	0	0	0
			2780	1753	485	523	1	18			
1	E	321	Total	C	N	O	P	S	0	0	0
			2537	1597	449	472	1	18			
1	G	316	Total	C	N	O	P	S	0	0	0
			2501	1577	438	469	1	16			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	MET	-	initiating methionine	UNP Q9Y697
A	33	GLY	-	expression tag	UNP Q9Y697
A	34	SER	-	expression tag	UNP Q9Y697
A	35	SER	-	expression tag	UNP Q9Y697
A	36	HIS	-	expression tag	UNP Q9Y697
A	37	HIS	-	expression tag	UNP Q9Y697
A	38	HIS	-	expression tag	UNP Q9Y697
A	39	HIS	-	expression tag	UNP Q9Y697
A	40	HIS	-	expression tag	UNP Q9Y697
A	41	HIS	-	expression tag	UNP Q9Y697
A	42	SER	-	expression tag	UNP Q9Y697
A	43	SER	-	expression tag	UNP Q9Y697
A	44	GLY	-	expression tag	UNP Q9Y697
A	45	LEU	-	expression tag	UNP Q9Y697
A	46	VAL	-	expression tag	UNP Q9Y697
A	47	PRO	-	expression tag	UNP Q9Y697
A	48	ARG	-	expression tag	UNP Q9Y697
A	49	GLY	-	expression tag	UNP Q9Y697
A	50	SER	-	expression tag	UNP Q9Y697
A	51	HIS	-	expression tag	UNP Q9Y697
A	52	MET	-	expression tag	UNP Q9Y697

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Chain	Residue	Modelled	Actual	Comment	Reference
A	53	LEU	-	expression tag	UNP Q9Y697
A	54	GLU	-	expression tag	UNP Q9Y697
A	55	MET	-	expression tag	UNP Q9Y697
C	32	MET	-	initiating methionine	UNP Q9Y697
C	33	GLY	-	expression tag	UNP Q9Y697
C	34	SER	-	expression tag	UNP Q9Y697
C	35	SER	-	expression tag	UNP Q9Y697
C	36	HIS	-	expression tag	UNP Q9Y697
C	37	HIS	-	expression tag	UNP Q9Y697
C	38	HIS	-	expression tag	UNP Q9Y697
C	39	HIS	-	expression tag	UNP Q9Y697
C	40	HIS	-	expression tag	UNP Q9Y697
C	41	HIS	-	expression tag	UNP Q9Y697
C	42	SER	-	expression tag	UNP Q9Y697
C	43	SER	-	expression tag	UNP Q9Y697
C	44	GLY	-	expression tag	UNP Q9Y697
C	45	LEU	-	expression tag	UNP Q9Y697
C	46	VAL	-	expression tag	UNP Q9Y697
C	47	PRO	-	expression tag	UNP Q9Y697
C	48	ARG	-	expression tag	UNP Q9Y697
C	49	GLY	-	expression tag	UNP Q9Y697
C	50	SER	-	expression tag	UNP Q9Y697
C	51	HIS	-	expression tag	UNP Q9Y697
C	52	MET	-	expression tag	UNP Q9Y697
C	53	LEU	-	expression tag	UNP Q9Y697
C	54	GLU	-	expression tag	UNP Q9Y697
C	55	MET	-	expression tag	UNP Q9Y697
E	32	MET	-	initiating methionine	UNP Q9Y697
E	33	GLY	-	expression tag	UNP Q9Y697
E	34	SER	-	expression tag	UNP Q9Y697
E	35	SER	-	expression tag	UNP Q9Y697
E	36	HIS	-	expression tag	UNP Q9Y697
E	37	HIS	-	expression tag	UNP Q9Y697
E	38	HIS	-	expression tag	UNP Q9Y697
E	39	HIS	-	expression tag	UNP Q9Y697
E	40	HIS	-	expression tag	UNP Q9Y697
E	41	HIS	-	expression tag	UNP Q9Y697
E	42	SER	-	expression tag	UNP Q9Y697
E	43	SER	-	expression tag	UNP Q9Y697
E	44	GLY	-	expression tag	UNP Q9Y697
E	45	LEU	-	expression tag	UNP Q9Y697
E	46	VAL	-	expression tag	UNP Q9Y697

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Chain	Residue	Modelled	Actual	Comment	Reference
E	47	PRO	-	expression tag	UNP Q9Y697
E	48	ARG	-	expression tag	UNP Q9Y697
E	49	GLY	-	expression tag	UNP Q9Y697
E	50	SER	-	expression tag	UNP Q9Y697
E	51	HIS	-	expression tag	UNP Q9Y697
E	52	MET	-	expression tag	UNP Q9Y697
E	53	LEU	-	expression tag	UNP Q9Y697
E	54	GLU	-	expression tag	UNP Q9Y697
E	55	MET	-	expression tag	UNP Q9Y697
G	32	MET	-	initiating methionine	UNP Q9Y697
G	33	GLY	-	expression tag	UNP Q9Y697
G	34	SER	-	expression tag	UNP Q9Y697
G	35	SER	-	expression tag	UNP Q9Y697
G	36	HIS	-	expression tag	UNP Q9Y697
G	37	HIS	-	expression tag	UNP Q9Y697
G	38	HIS	-	expression tag	UNP Q9Y697
G	39	HIS	-	expression tag	UNP Q9Y697
G	40	HIS	-	expression tag	UNP Q9Y697
G	41	HIS	-	expression tag	UNP Q9Y697
G	42	SER	-	expression tag	UNP Q9Y697
G	43	SER	-	expression tag	UNP Q9Y697
G	44	GLY	-	expression tag	UNP Q9Y697
G	45	LEU	-	expression tag	UNP Q9Y697
G	46	VAL	-	expression tag	UNP Q9Y697
G	47	PRO	-	expression tag	UNP Q9Y697
G	48	ARG	-	expression tag	UNP Q9Y697
G	49	GLY	-	expression tag	UNP Q9Y697
G	50	SER	-	expression tag	UNP Q9Y697
G	51	HIS	-	expression tag	UNP Q9Y697
G	52	MET	-	expression tag	UNP Q9Y697
G	53	LEU	-	expression tag	UNP Q9Y697
G	54	GLU	-	expression tag	UNP Q9Y697
G	55	MET	-	expression tag	UNP Q9Y697

- Molecule 2 is a protein called LYR motif-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	0	0
			634	395	127	111	1			
2	D	80	Total	C	N	O	S	0	0	0
			667	419	132	115	1			
2	F	75	Total	C	N	O	S	0	0	0
			626	391	126	108	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	77	639	398	128	112	1	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	ALA	SER	engineered mutation	UNP Q9HD34
D	11	ALA	SER	engineered mutation	UNP Q9HD34
F	11	ALA	SER	engineered mutation	UNP Q9HD34
H	11	ALA	SER	engineered mutation	UNP Q9HD34

- Molecule 3 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	76	591	365	92	133	1	0	0	0
3	J	75	585	362	91	131	1	0	0	0
3	K	69	539	335	81	122	1	0	0	0
3	L	71	554	345	83	125	1	0	0	0

- Molecule 4 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).
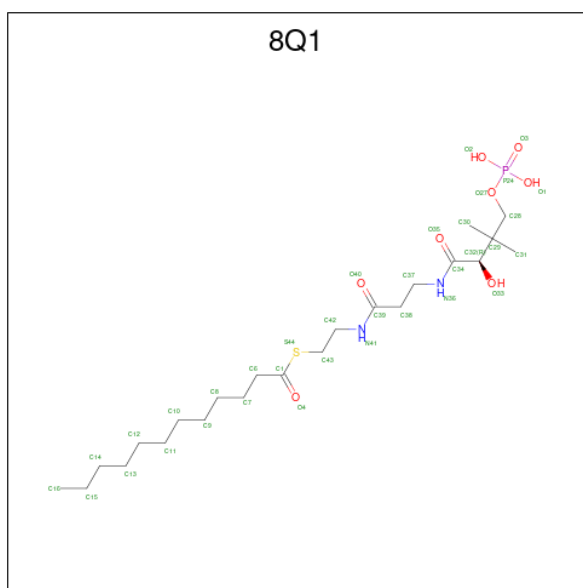
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	I	1	Total	C	N	O	P	S		0	0
			34	23	2	7	1	1			
4	J	1	Total	C	N	O	P	S		0	0
			34	23	2	7	1	1			
4	K	1	Total	C	N	O	P	S		0	0
			34	23	2	7	1	1			
4	L	1	Total	C	N	O	P	S		0	0
			34	23	2	7	1	1			

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: Cysteine desulfurase, mitochondrial
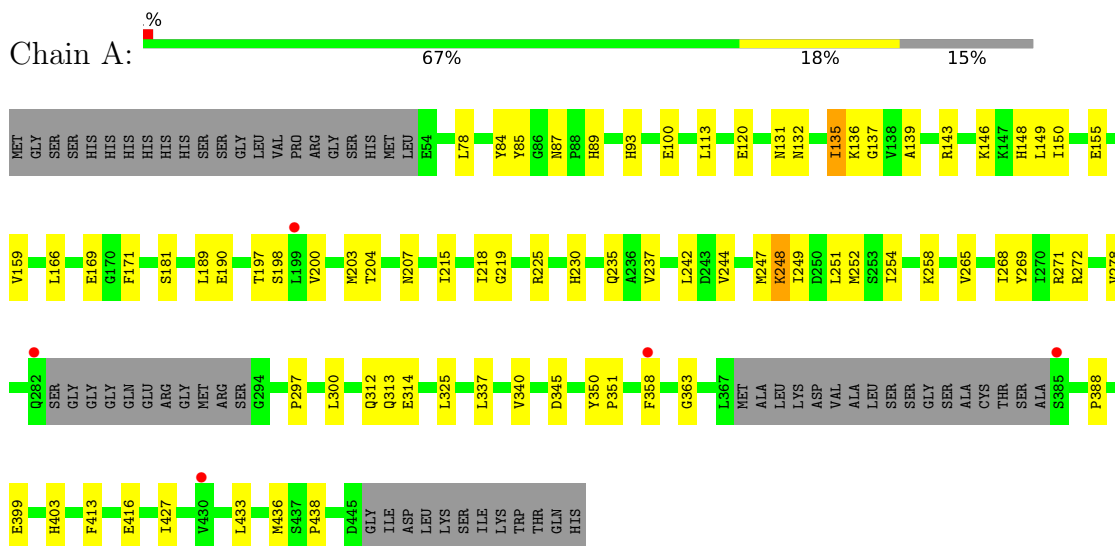
Chain A:

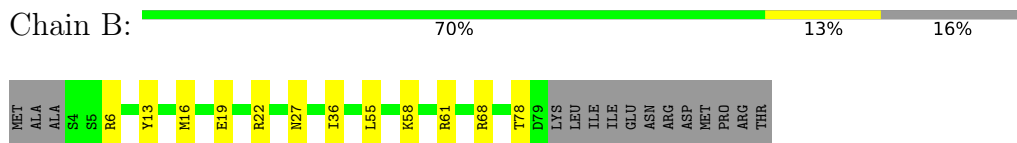• Molecule 1: Cysteine desulfurase, mitochondrial

Chain C:

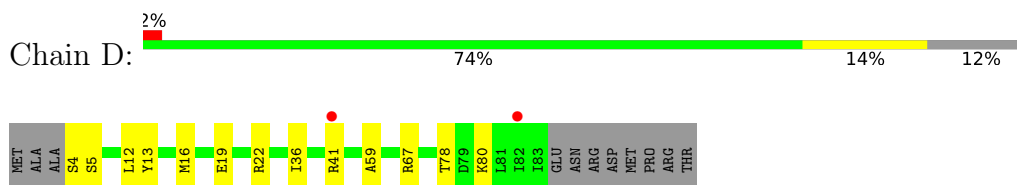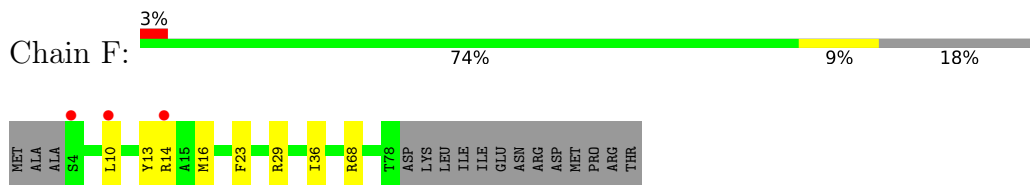• Molecule 1: Cysteine desulfurase, mitochondrial

Chain E:

2%

61%   14%   25%

- Molecule 1: Cysteine desulfurase, mitochondrial

Chain G:

4%

60%   13%   26%

- Molecule 2: LYR motif-containing protein 4

Chain B:

70%   13%   16%

- Molecule 2: LYR motif-containing protein 4

Chain D:

2%

74%   14%   12%

• Molecule 2: LYR motif-containing protein 4

Chain F:

• Molecule 2: LYR motif-containing protein 4

Chain H:

• Molecule 3: Acyl carrier protein

Chain I:

• Molecule 3: Acyl carrier protein

Chain J:

• Molecule 3: Acyl carrier protein

Chain K:

• Molecule 3: Acyl carrier protein

Chain L:
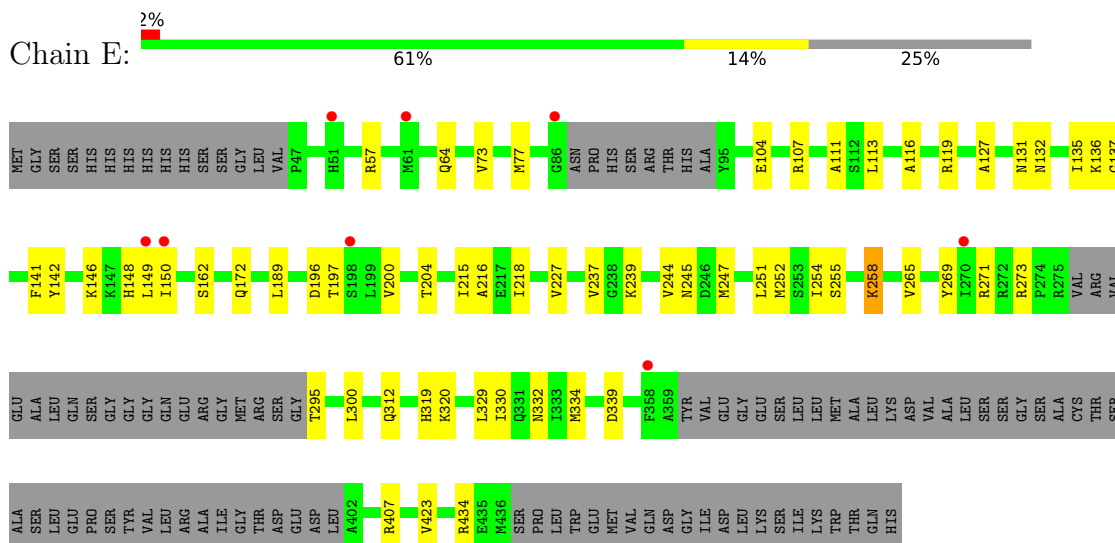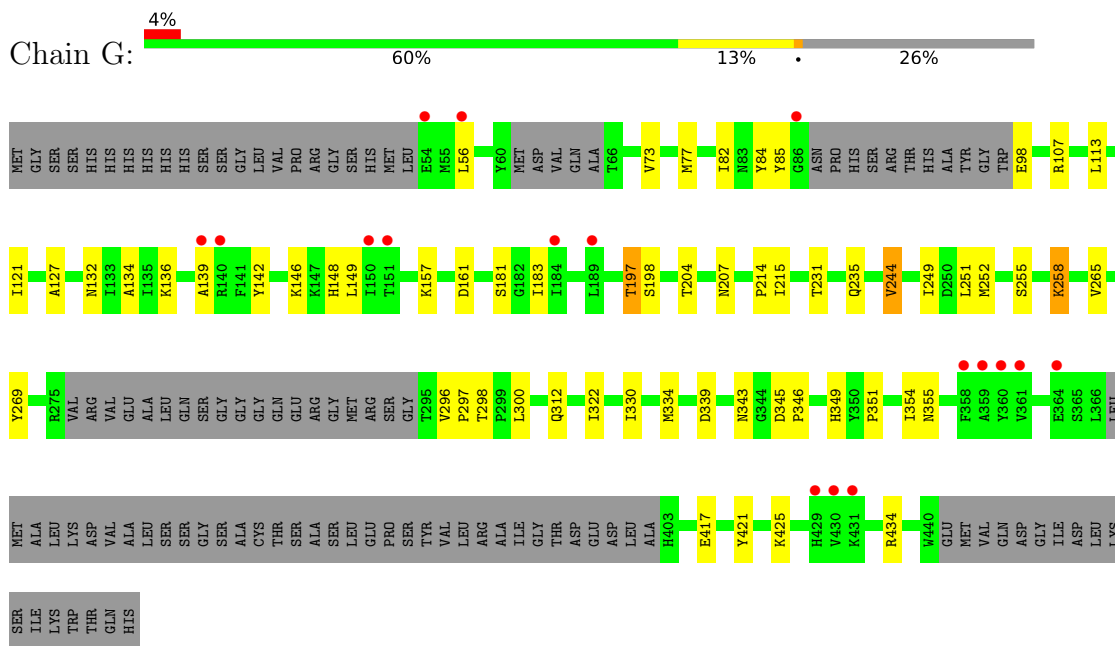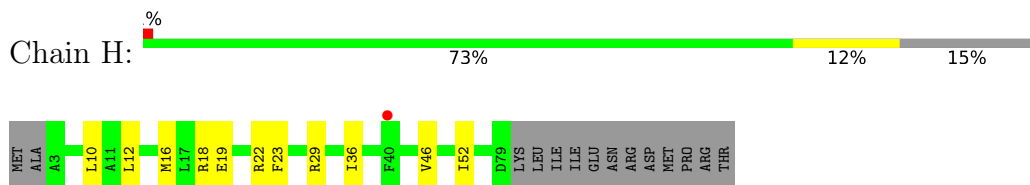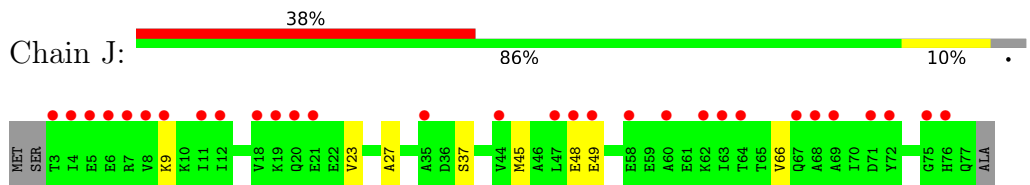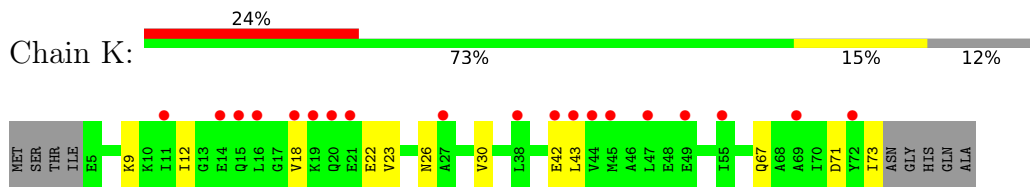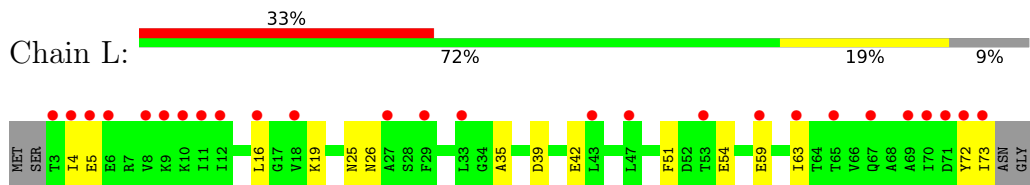
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.48Å 147.78Å 168.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.83 – 3.09 47.83 – 3.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.83-3.09) 99.9 (47.83-3.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 3.07Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.212 , 0.259 0.212 , 0.259	Depositor DCC
R_{free} test set	2000 reflections (3.45%)	wwPDB-VP
Wilson B-factor (Å^2)	103.5	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 75.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	15666	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: LLP, 8Q1

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	0.25	0/2905	0.44	0/3929
1	C	0.24	0/2802	0.43	0/3785
1	E	0.25	0/2557	0.44	0/3449
1	G	0.25	0/2519	0.44	0/3399
2	B	0.24	0/642	0.37	0/860
2	D	0.25	0/675	0.38	0/904
2	F	0.25	0/634	0.39	0/849
2	H	0.24	0/647	0.38	0/867
3	I	0.24	0/595	0.43	0/805
3	J	0.24	0/589	0.41	0/797
3	K	0.24	0/542	0.40	0/733
3	L	0.24	0/557	0.42	0/754
All	All	0.25	0/15664	0.42	0/21131

There are no bond length outliers.

There are no bond angle outliers.

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	2877	0	2883	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2780	0	2807	52	0
1	E	2537	0	2561	36	0
1	G	2501	0	2523	33	0
2	B	634	0	656	8	0
2	D	667	0	702	10	0
2	F	626	0	652	7	0
2	H	639	0	661	7	0
3	I	591	0	565	12	0
3	J	585	0	560	6	0
3	K	539	0	518	5	0
3	L	554	0	536	8	0
4	I	34	0	0	0	0
4	J	34	0	0	0	0
4	K	34	0	0	2	0
4	L	34	0	0	0	0
All	All	15666	0	15624	214	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 7.

The worst 5 of 214 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:181:SER:HB2	1:A:345:ASP:HB2	1.61	0.82
1:G:181:SER:HB2	1:G:345:ASP:HB2	1.63	0.80
1:A:363:GLY:HA3	1:A:438:PRO:HG3	1.67	0.77
1:E:119:ARG:NH2	1:E:273:ARG:O	2.22	0.73
1:A:337:LEU:HD11	1:A:427:ILE:HA	1.70	0.73

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	357/426 (84%)	339 (95%)	14 (4%)	4 (1%)	14	46
1	C	343/426 (80%)	326 (95%)	15 (4%)	2 (1%)	25	59
1	E	312/426 (73%)	291 (93%)	21 (7%)	0	100	100
1	G	305/426 (72%)	293 (96%)	12 (4%)	0	100	100
2	B	74/91 (81%)	73 (99%)	1 (1%)	0	100	100
2	D	78/91 (86%)	76 (97%)	2 (3%)	0	100	100
2	F	73/91 (80%)	70 (96%)	3 (4%)	0	100	100
2	H	75/91 (82%)	73 (97%)	2 (3%)	0	100	100
3	I	74/78 (95%)	71 (96%)	3 (4%)	0	100	100
3	J	73/78 (94%)	68 (93%)	5 (7%)	0	100	100
3	K	67/78 (86%)	62 (92%)	4 (6%)	1 (2%)	10	39
3	L	69/78 (88%)	63 (91%)	5 (7%)	1 (1%)	11	40
All	All	1900/2380 (80%)	1805 (95%)	87 (5%)	8 (0%)	34	69

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	248	LYS
3	L	26	ASN
1	A	388	PRO
3	K	71	ASP
1	A	93	HIS

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	314/363 (86%)	313 (100%)	1 (0%)	92	96
1	C	303/363 (84%)	299 (99%)	4 (1%)	69	87
1	E	276/363 (76%)	274 (99%)	2 (1%)	84	93
1	G	274/363 (76%)	271 (99%)	3 (1%)	73	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	67/80 (84%)	66 (98%)	1 (2%)	65	85
2	D	71/80 (89%)	70 (99%)	1 (1%)	67	86
2	F	66/80 (82%)	66 (100%)	0	100	100
2	H	67/80 (84%)	67 (100%)	0	100	100
3	I	66/67 (98%)	65 (98%)	1 (2%)	65	85
3	J	65/67 (97%)	65 (100%)	0	100	100
3	K	60/67 (90%)	58 (97%)	2 (3%)	38	69
3	L	62/67 (92%)	61 (98%)	1 (2%)	62	84
All	All	1691/2040 (83%)	1675 (99%)	16 (1%)	78	91

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	73	ILE
3	K	30	VAL
1	E	295	THR
3	I	65	THR
1	E	149	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	331	GLN
3	J	74	ASN
3	K	67	GLN
3	K	20	GLN
1	C	235	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	#$|Z| > 2$
1	LLP	G	258	1	23,24,25	2.67	6 (26%)	25,32,34	1.26	3 (12%)
1	LLP	A	258	1	23,24,25	2.64	6 (26%)	25,32,34	1.39	4 (16%)
1	LLP	C	258	1	23,24,25	2.65	7 (30%)	25,32,34	1.22	4 (16%)
1	LLP	E	258	1	23,24,25	2.67	5 (21%)	25,32,34	1.31	3 (12%)

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
1	LLP	G	258	1	-	10/16/17/19	0/1/1/1
1	LLP	A	258	1	-	8/16/17/19	0/1/1/1
1	LLP	C	258	1	-	10/16/17/19	0/1/1/1
1	LLP	E	258	1	-	11/16/17/19	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	258	LLP	C4-C4'	8.24	1.62	1.46
1	G	258	LLP	C4-C4'	8.16	1.62	1.46
1	A	258	LLP	C4-C4'	8.16	1.62	1.46
1	C	258	LLP	C4-C4'	8.10	1.62	1.46
1	C	258	LLP	C4'-NZ	4.97	1.43	1.27

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	258	LLP	CE-NZ-C4'	-3.62	107.77	118.90
1	A	258	LLP	C4-C4'-NZ	-3.36	108.89	124.31
1	C	258	LLP	C4-C4'-NZ	-3.17	109.76	124.31
1	E	258	LLP	C4-C4'-NZ	-3.08	110.15	124.31
1	G	258	LLP	C4-C4'-NZ	-2.96	110.73	124.31

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	258	LLP	C4-C4'-NZ-CE
1	A	258	LLP	C5'-OP4-P-OP2
1	A	258	LLP	C5'-OP4-P-OP3
1	C	258	LLP	C4-C4'-NZ-CE
1	C	258	LLP	C5'-OP4-P-OP2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	258	LLP	2	0
1	C	258	LLP	1	0
1	E	258	LLP	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
4	8Q1	K	101	3	27,33,34	0.85	1 (3%)	32,40,43	1.38	4 (12%)
4	8Q1	J	101	3	27,33,34	0.85	1 (3%)	32,40,43	1.49	4 (12%)
4	8Q1	I	101	3	27,33,34	0.83	1 (3%)	32,40,43	1.67	5 (15%)
4	8Q1	L	101	3	27,33,34	0.85	1 (3%)	32,40,43	1.48	4 (12%)

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
4	8Q1	K	101	3	-	8/38/40/41	-
4	8Q1	J	101	3	-	18/38/40/41	-
4	8Q1	I	101	3	-	12/38/40/41	-
4	8Q1	L	101	3	-	9/38/40/41	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	101	8Q1	C1-S44	-3.75	1.67	1.76
4	K	101	8Q1	C1-S44	-3.65	1.67	1.76
4	J	101	8Q1	C1-S44	-3.63	1.67	1.76
4	I	101	8Q1	C1-S44	-3.42	1.67	1.76

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	101	8Q1	C6-C1-S44	6.39	120.90	113.46
4	J	101	8Q1	C6-C1-S44	6.09	120.55	113.46
4	L	101	8Q1	C6-C1-S44	5.78	120.19	113.46
4	K	101	8Q1	C6-C1-S44	5.51	119.87	113.46
4	I	101	8Q1	O4-C1-C6	-3.90	119.38	123.99

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	101	8Q1	O27-C28-C29-C32
4	I	101	8Q1	C32-C34-N36-C37
4	I	101	8Q1	O35-C34-N36-C37
4	I	101	8Q1	C42-C43-S44-C1
4	J	101	8Q1	O4-C1-S44-C43

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	101	8Q1	2	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 8Q1 K 101

Bond lengths — Bond angles — Torsions — Rings

Ligand 8Q1 J 101

Bond lengths — Bond angles — Torsions — Rings

Ligand 8Q1 I 101

Bond lengths

Bond angles

Torsions

Rings

Ligand 8Q1 L 101

Bond lengths

Bond angles

Torsions

Rings
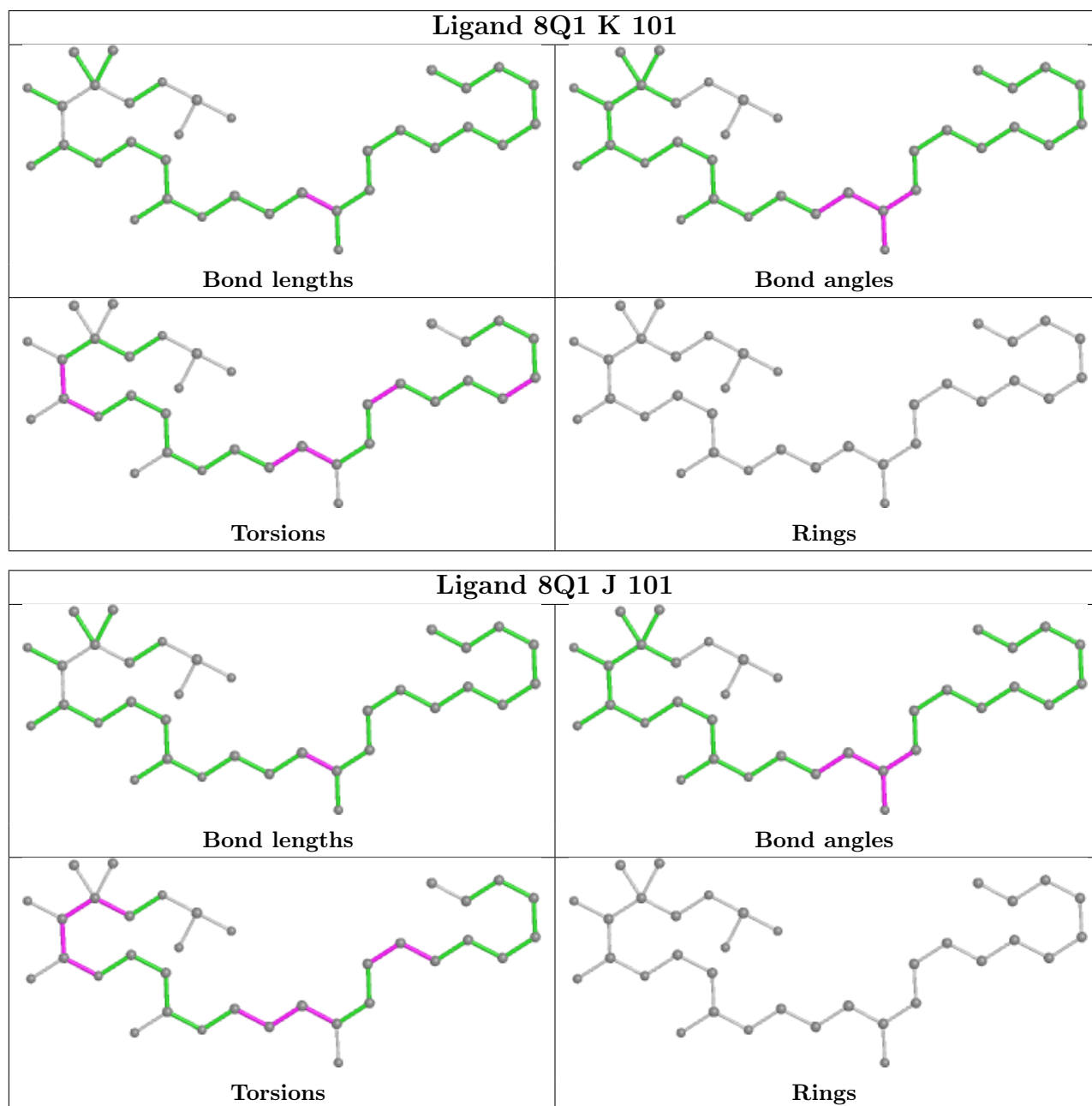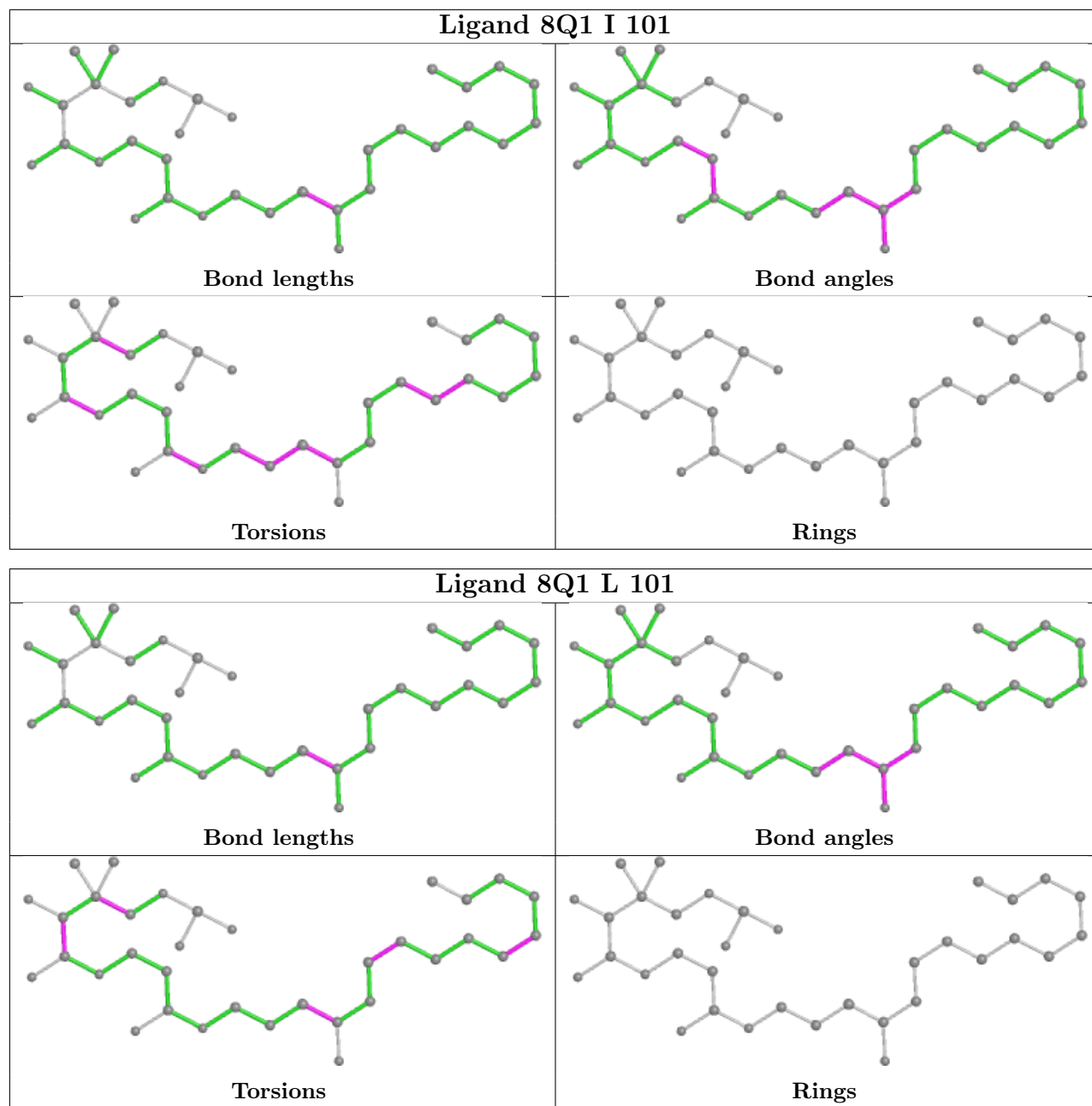
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	363/426 (85%)	0.18	5 (1%)	75	56	65, 107, 165, 234	0
1	C	351/426 (82%)	0.58	34 (9%)	7	2	76, 148, 205, 237	0
1	E	320/426 (75%)	0.21	8 (2%)	57	34	54, 91, 161, 208	0
1	G	315/426 (73%)	0.29	17 (5%)	25	12	72, 106, 157, 208	0
2	B	76/91 (83%)	0.08	0	100	100	72, 104, 158, 176	0
2	D	80/91 (87%)	0.05	2 (2%)	57	34	74, 107, 163, 201	0
2	F	75/91 (82%)	0.32	3 (4%)	38	19	60, 92, 145, 163	0
2	H	77/91 (84%)	0.06	1 (1%)	77	59	67, 103, 156, 193	0
3	I	76/78 (97%)	0.62	7 (9%)	9	3	82, 152, 204, 225	0
3	J	75/78 (96%)	1.89	30 (40%)	0	0	127, 194, 246, 252	0
3	K	69/78 (88%)	1.26	19 (27%)	0	0	145, 206, 230, 242	0
3	L	71/78 (91%)	1.64	26 (36%)	0	0	127, 216, 244, 251	0
All	All	1948/2380 (81%)	0.44	152 (7%)	13	5	54, 117, 213, 252	0

The worst 5 of 152 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	27	ALA	10.2
3	J	47	LEU	7.4
3	J	3	THR	6.7
3	K	72	TYR	6.6
3	K	15	GLN	6.5

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

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

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
1	LLP	A	258	24/25	0.90	0.27	67,105,136,137	0
1	LLP	G	258	24/25	0.93	0.26	68,99,121,132	0
1	LLP	E	258	24/25	0.95	0.23	52,87,106,122	0
1	LLP	C	258	24/25	0.95	0.21	90,146,172,177	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	8Q1	K	101	34/35	0.87	0.41	73,118,145,161	0
4	8Q1	L	101	34/35	0.91	0.33	70,104,138,163	0
4	8Q1	I	101	34/35	0.93	0.47	52,90,129,154	0
4	8Q1	J	101	34/35	0.93	0.39	54,120,156,159	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 8Q1 K 101:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
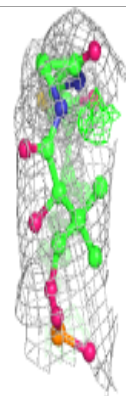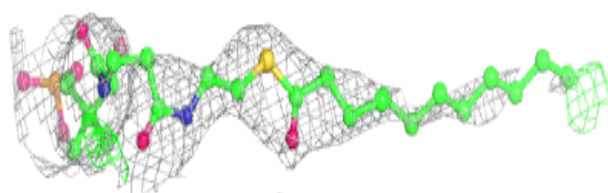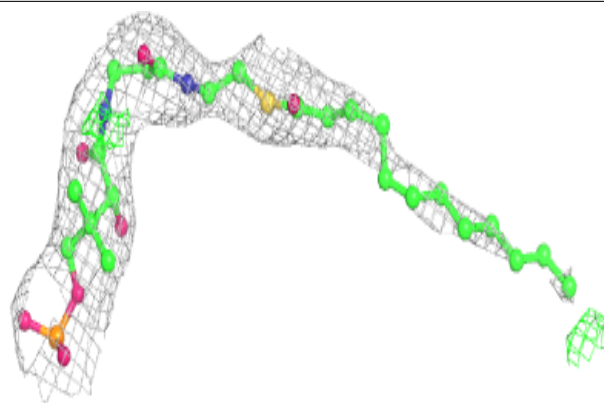$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
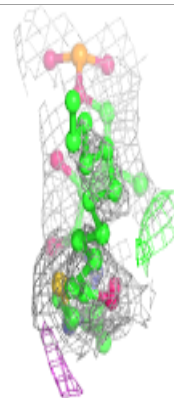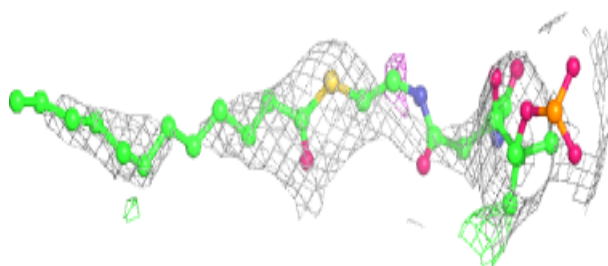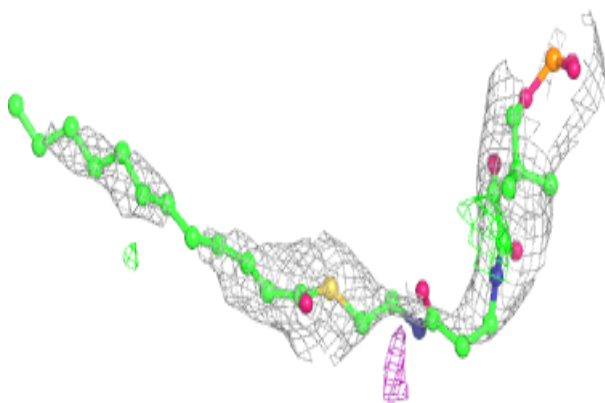
Electron density around 8Q1 L 101:

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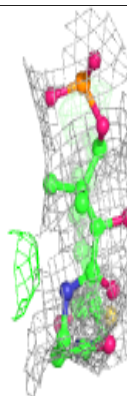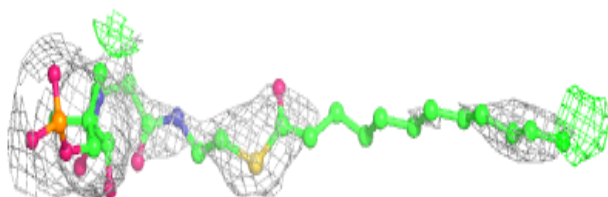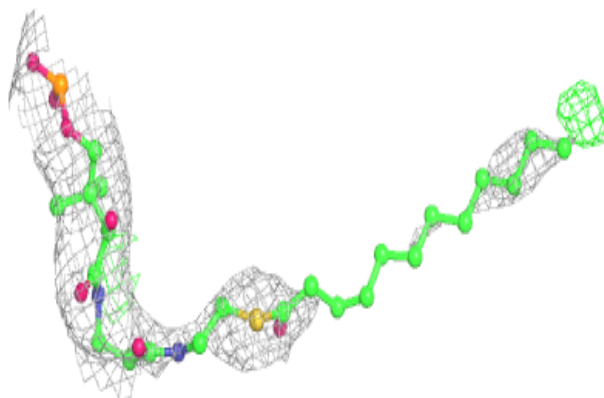$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
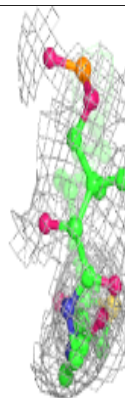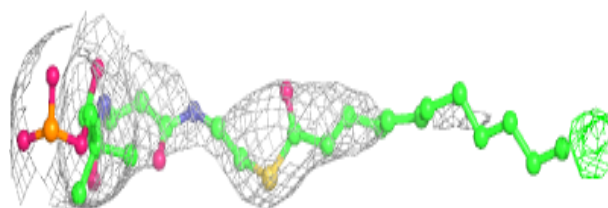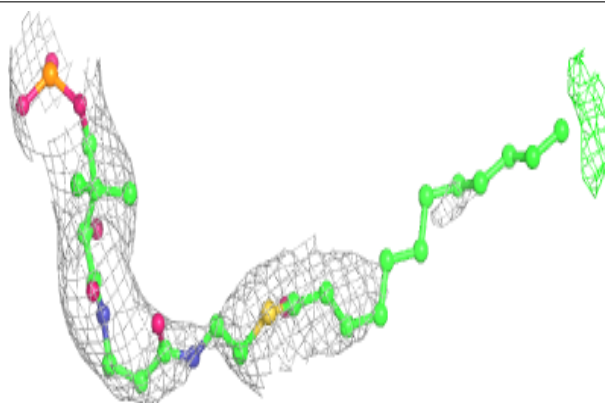
Electron density around 8Q1 I 101:

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

Electron density around 8Q1 J 101:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.