



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 09:08 PM EDT

PDB ID : 5O68
Title : Crystal Structure of the Pseudomonas functional amyloid secretion protein FapF - R157A mutant
Authors : Rouse, S.L.; Hare, S.; Lambert, S.; Morgan, R.M.L.; Hawthorne, W.J.; Berry, J.; Matthews, S.J.
Deposited on : 2017-06-05
Resolution : 3.08 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

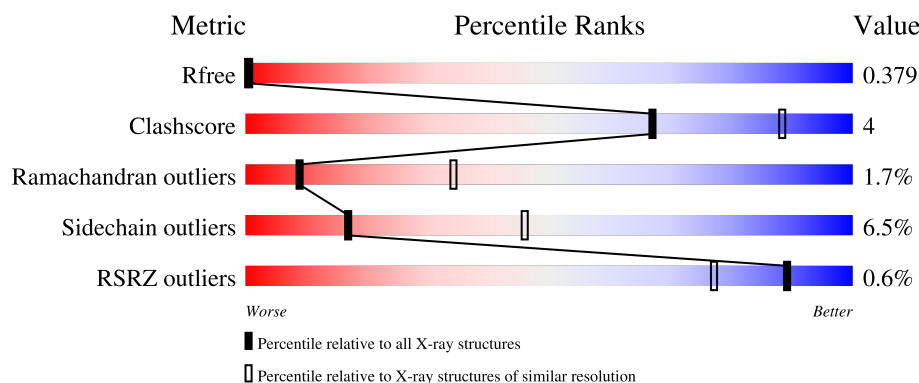
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.08 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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	334	
1	B	334	
1	C	334	
1	D	334	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	334	<div><div>%</div><div><div></div><div>69%</div><div>12%</div><div>18%</div></div></div>
1	F	334	<div><div>2%</div><div><div></div><div>65%</div><div>10%</div><div>24%</div></div></div>
1	G	334	<div><div><div></div><div>69%</div><div>11%</div><div>19%</div></div></div>
1	H	334	<div><div><div></div><div>71%</div><div>10%</div><div>19%</div></div></div>
1	I	334	<div><div><div></div><div>66%</div><div>10%</div><div>23%</div></div></div>
1	J	334	<div><div><div></div><div>69%</div><div>10%</div><div>20%</div></div></div>
1	K	334	<div><div><div></div><div>67%</div><div>13%</div><div>19%</div></div></div>
1	L	334	<div><div><div></div><div>66%</div><div>11%</div><div>23%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23772 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 FapF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2001	1276	322	397	6			
1	B	274	Total	C	N	O	S	0	0	0
			2037	1299	329	403	6			
1	C	262	Total	C	N	O	S	0	0	0
			1922	1229	315	372	6			
1	D	271	Total	C	N	O	S	0	0	0
			2013	1291	325	392	5			
1	E	273	Total	C	N	O	S	0	0	0
			2028	1294	329	400	5			
1	F	254	Total	C	N	O	S	0	0	0
			1860	1192	304	358	6			
1	G	271	Total	C	N	O	S	0	0	0
			2014	1294	323	391	6			
1	H	272	Total	C	N	O	S	0	0	0
			1982	1261	321	394	6			
1	I	256	Total	C	N	O	S	0	0	0
			1895	1212	310	368	5			
1	J	268	Total	C	N	O	S	0	0	0
			1993	1283	319	385	6			
1	K	272	Total	C	N	O	S	0	0	0
			2016	1287	328	396	5			
1	L	258	Total	C	N	O	S	0	0	0
			1904	1218	312	368	6			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	THR	-	expression tag	UNP C4IN73
A	74	SER	-	expression tag	UNP C4IN73
A	75	HIS	-	expression tag	UNP C4IN73
A	76	HIS	-	expression tag	UNP C4IN73
A	77	HIS	-	expression tag	UNP C4IN73

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	HIS	-	expression tag	UNP C4IN73
A	79	HIS	-	expression tag	UNP C4IN73
A	80	HIS	-	expression tag	UNP C4IN73
A	81	GLY	-	expression tag	UNP C4IN73
A	82	THR	-	expression tag	UNP C4IN73
A	157	ALA	ARG	engineered mutation	UNP C4IN73
A	273	MET	LEU	conflict	UNP C4IN73
B	73	THR	-	expression tag	UNP C4IN73
B	74	SER	-	expression tag	UNP C4IN73
B	75	HIS	-	expression tag	UNP C4IN73
B	76	HIS	-	expression tag	UNP C4IN73
B	77	HIS	-	expression tag	UNP C4IN73
B	78	HIS	-	expression tag	UNP C4IN73
B	79	HIS	-	expression tag	UNP C4IN73
B	80	HIS	-	expression tag	UNP C4IN73
B	81	GLY	-	expression tag	UNP C4IN73
B	82	THR	-	expression tag	UNP C4IN73
B	157	ALA	ARG	engineered mutation	UNP C4IN73
B	273	MET	LEU	conflict	UNP C4IN73
C	73	THR	-	expression tag	UNP C4IN73
C	74	SER	-	expression tag	UNP C4IN73
C	75	HIS	-	expression tag	UNP C4IN73
C	76	HIS	-	expression tag	UNP C4IN73
C	77	HIS	-	expression tag	UNP C4IN73
C	78	HIS	-	expression tag	UNP C4IN73
C	79	HIS	-	expression tag	UNP C4IN73
C	80	HIS	-	expression tag	UNP C4IN73
C	81	GLY	-	expression tag	UNP C4IN73
C	82	THR	-	expression tag	UNP C4IN73
C	157	ALA	ARG	engineered mutation	UNP C4IN73
C	273	MET	LEU	conflict	UNP C4IN73
D	73	THR	-	expression tag	UNP C4IN73
D	74	SER	-	expression tag	UNP C4IN73
D	75	HIS	-	expression tag	UNP C4IN73
D	76	HIS	-	expression tag	UNP C4IN73
D	77	HIS	-	expression tag	UNP C4IN73
D	78	HIS	-	expression tag	UNP C4IN73
D	79	HIS	-	expression tag	UNP C4IN73
D	80	HIS	-	expression tag	UNP C4IN73
D	81	GLY	-	expression tag	UNP C4IN73
D	82	THR	-	expression tag	UNP C4IN73
D	157	ALA	ARG	engineered mutation	UNP C4IN73

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	273	MET	LEU	conflict	UNP C4IN73
E	73	THR	-	expression tag	UNP C4IN73
E	74	SER	-	expression tag	UNP C4IN73
E	75	HIS	-	expression tag	UNP C4IN73
E	76	HIS	-	expression tag	UNP C4IN73
E	77	HIS	-	expression tag	UNP C4IN73
E	78	HIS	-	expression tag	UNP C4IN73
E	79	HIS	-	expression tag	UNP C4IN73
E	80	HIS	-	expression tag	UNP C4IN73
E	81	GLY	-	expression tag	UNP C4IN73
E	82	THR	-	expression tag	UNP C4IN73
E	157	ALA	ARG	engineered mutation	UNP C4IN73
E	273	MET	LEU	conflict	UNP C4IN73
F	73	THR	-	expression tag	UNP C4IN73
F	74	SER	-	expression tag	UNP C4IN73
F	75	HIS	-	expression tag	UNP C4IN73
F	76	HIS	-	expression tag	UNP C4IN73
F	77	HIS	-	expression tag	UNP C4IN73
F	78	HIS	-	expression tag	UNP C4IN73
F	79	HIS	-	expression tag	UNP C4IN73
F	80	HIS	-	expression tag	UNP C4IN73
F	81	GLY	-	expression tag	UNP C4IN73
F	82	THR	-	expression tag	UNP C4IN73
F	157	ALA	ARG	engineered mutation	UNP C4IN73
F	273	MET	LEU	conflict	UNP C4IN73
G	73	THR	-	expression tag	UNP C4IN73
G	74	SER	-	expression tag	UNP C4IN73
G	75	HIS	-	expression tag	UNP C4IN73
G	76	HIS	-	expression tag	UNP C4IN73
G	77	HIS	-	expression tag	UNP C4IN73
G	78	HIS	-	expression tag	UNP C4IN73
G	79	HIS	-	expression tag	UNP C4IN73
G	80	HIS	-	expression tag	UNP C4IN73
G	81	GLY	-	expression tag	UNP C4IN73
G	82	THR	-	expression tag	UNP C4IN73
G	157	ALA	ARG	engineered mutation	UNP C4IN73
G	273	MET	LEU	conflict	UNP C4IN73
H	73	THR	-	expression tag	UNP C4IN73
H	74	SER	-	expression tag	UNP C4IN73
H	75	HIS	-	expression tag	UNP C4IN73
H	76	HIS	-	expression tag	UNP C4IN73
H	77	HIS	-	expression tag	UNP C4IN73

Continued on next page...

Continued from previous page...

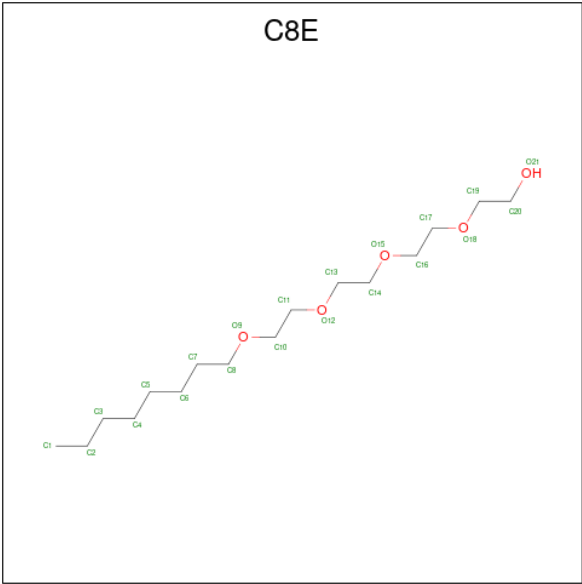
Chain	Residue	Modelled	Actual	Comment	Reference
H	78	HIS	-	expression tag	UNP C4IN73
H	79	HIS	-	expression tag	UNP C4IN73
H	80	HIS	-	expression tag	UNP C4IN73
H	81	GLY	-	expression tag	UNP C4IN73
H	82	THR	-	expression tag	UNP C4IN73
H	157	ALA	ARG	engineered mutation	UNP C4IN73
H	273	MET	LEU	conflict	UNP C4IN73
I	73	THR	-	expression tag	UNP C4IN73
I	74	SER	-	expression tag	UNP C4IN73
I	75	HIS	-	expression tag	UNP C4IN73
I	76	HIS	-	expression tag	UNP C4IN73
I	77	HIS	-	expression tag	UNP C4IN73
I	78	HIS	-	expression tag	UNP C4IN73
I	79	HIS	-	expression tag	UNP C4IN73
I	80	HIS	-	expression tag	UNP C4IN73
I	81	GLY	-	expression tag	UNP C4IN73
I	82	THR	-	expression tag	UNP C4IN73
I	157	ALA	ARG	engineered mutation	UNP C4IN73
I	273	MET	LEU	conflict	UNP C4IN73
J	73	THR	-	expression tag	UNP C4IN73
J	74	SER	-	expression tag	UNP C4IN73
J	75	HIS	-	expression tag	UNP C4IN73
J	76	HIS	-	expression tag	UNP C4IN73
J	77	HIS	-	expression tag	UNP C4IN73
J	78	HIS	-	expression tag	UNP C4IN73
J	79	HIS	-	expression tag	UNP C4IN73
J	80	HIS	-	expression tag	UNP C4IN73
J	81	GLY	-	expression tag	UNP C4IN73
J	82	THR	-	expression tag	UNP C4IN73
J	157	ALA	ARG	engineered mutation	UNP C4IN73
J	273	MET	LEU	conflict	UNP C4IN73
K	73	THR	-	expression tag	UNP C4IN73
K	74	SER	-	expression tag	UNP C4IN73
K	75	HIS	-	expression tag	UNP C4IN73
K	76	HIS	-	expression tag	UNP C4IN73
K	77	HIS	-	expression tag	UNP C4IN73
K	78	HIS	-	expression tag	UNP C4IN73
K	79	HIS	-	expression tag	UNP C4IN73
K	80	HIS	-	expression tag	UNP C4IN73
K	81	GLY	-	expression tag	UNP C4IN73
K	82	THR	-	expression tag	UNP C4IN73
K	157	ALA	ARG	engineered mutation	UNP C4IN73

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	273	MET	LEU	conflict	UNP C4IN73
L	73	THR	-	expression tag	UNP C4IN73
L	74	SER	-	expression tag	UNP C4IN73
L	75	HIS	-	expression tag	UNP C4IN73
L	76	HIS	-	expression tag	UNP C4IN73
L	77	HIS	-	expression tag	UNP C4IN73
L	78	HIS	-	expression tag	UNP C4IN73
L	79	HIS	-	expression tag	UNP C4IN73
L	80	HIS	-	expression tag	UNP C4IN73
L	81	GLY	-	expression tag	UNP C4IN73
L	82	THR	-	expression tag	UNP C4IN73
L	157	ALA	ARG	engineered mutation	UNP C4IN73
L	273	MET	LEU	conflict	UNP C4IN73

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



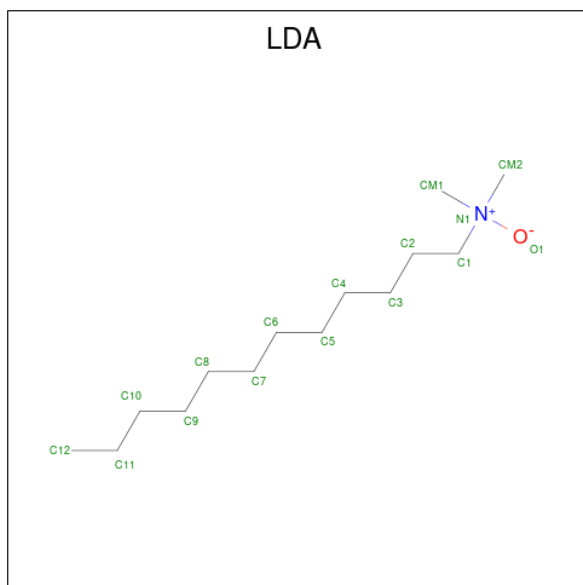
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 21 16 5	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C O 12 8 4	0	0
2	C	1	Total C O 9 6 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			11	10	1		

- Molecule 3 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

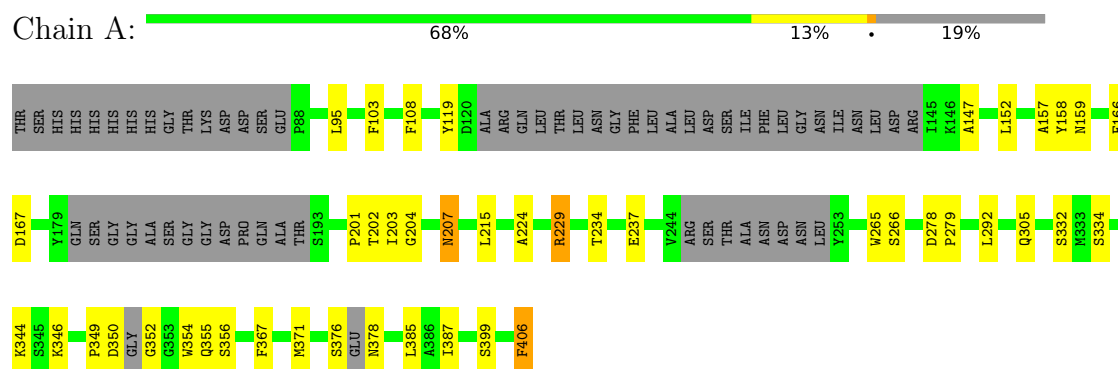


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	10	1	1		
3	B	1	Total	C	N	O	0	0
			9	7	1	1		
3	C	1	Total	C	N	O	0	0
			9	7	1	1		
3	I	1	Total	C	N	O	0	0
			16	14	1	1		

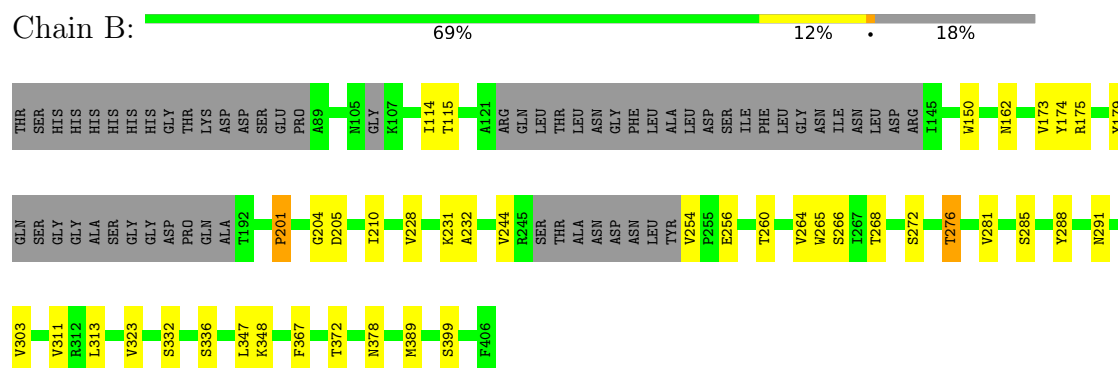
3 Residue-property plots [i](#)

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.

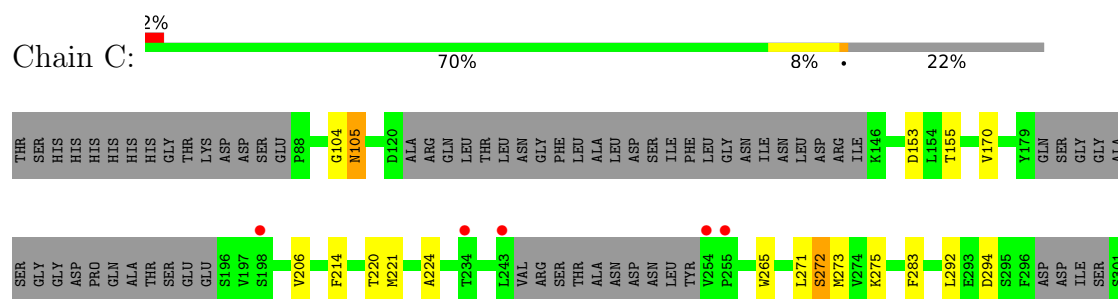
• Molecule 1: FapF

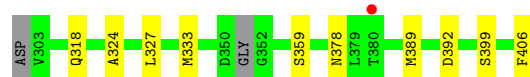


• Molecule 1: FapF

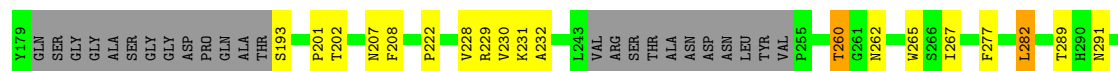
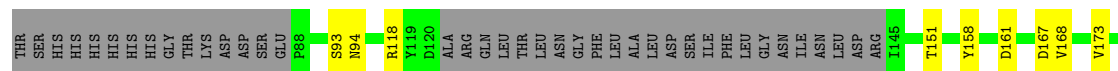


• Molecule 1: FapF

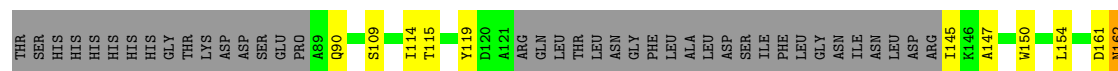




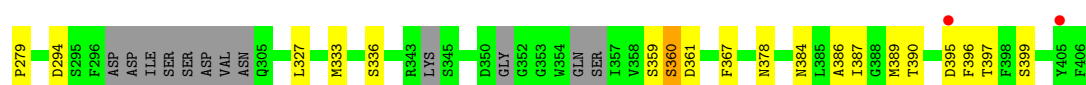
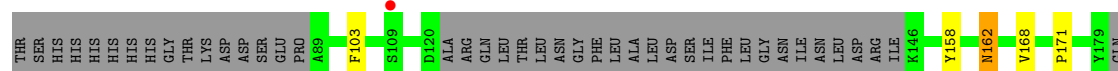
• Molecule 1: FapF



• Molecule 1: FapF

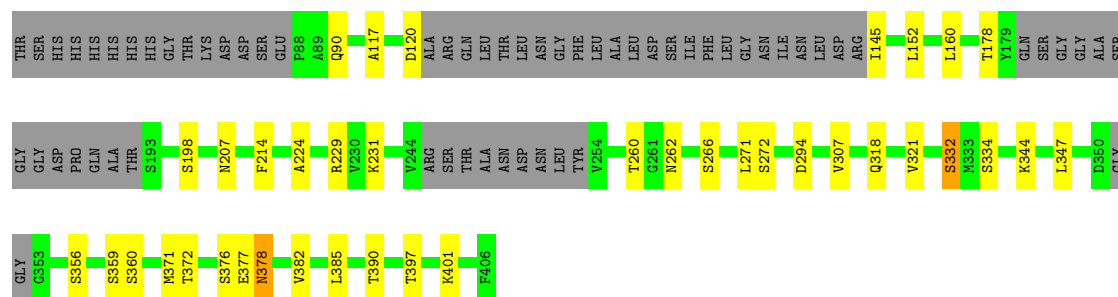


• Molecule 1: FapF



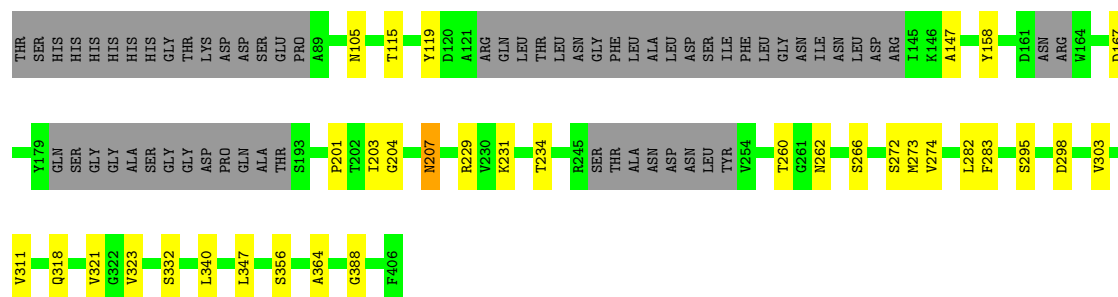
• Molecule 1: FapF





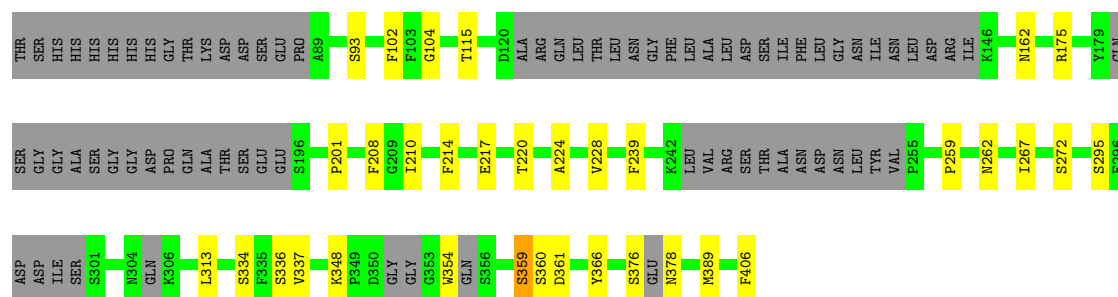
- Molecule 1: FapF

Chain H: 71% 10% 19%



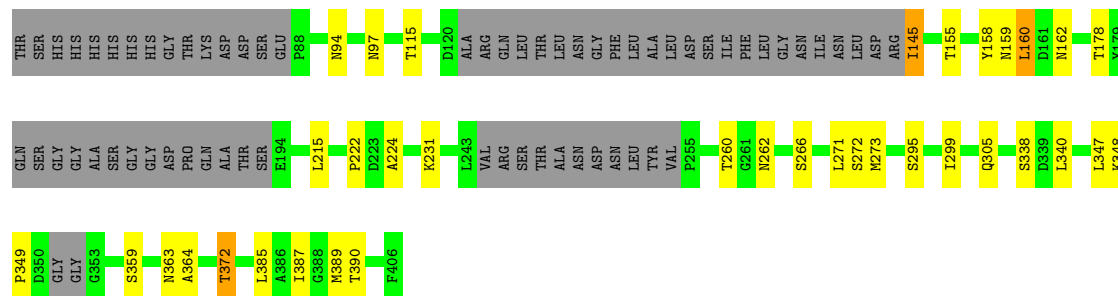
- Molecule 1: FapF

Chain I: 66% 10% 23%



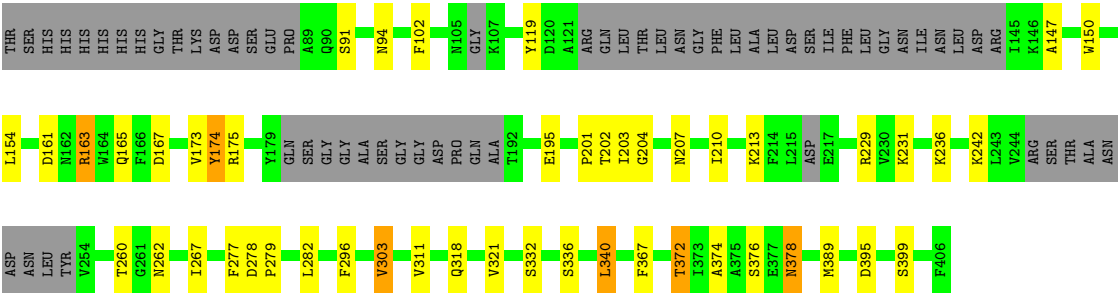
- Molecule 1: FapF

Chain J: 69% 10% 20%



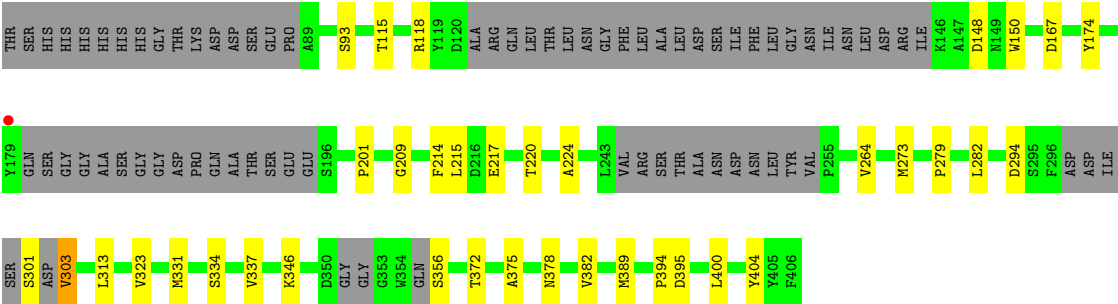
- Molecule 1: FapF

Chain K: 67% 13% 19%



● Molecule 1: FapF

Chain L: 66% 11% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.59Å 125.71Å 142.67Å 87.09° 84.70° 89.92°	Depositor
Resolution (Å)	91.73 – 3.08 91.73 – 3.08	Depositor EDS
% Data completeness (in resolution range)	96.4 (91.73-3.08) 96.5 (91.73-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.319 , 0.369 0.334 , 0.379	Depositor DCC
R_{free} test set	4983 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.038 for -h,k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	23772	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 80.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1929e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: C8E, LDA

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	0.58	0/2047	0.76	3/2789 (0.1%)
1	B	0.57	0/2083	0.75	0/2834
1	C	0.58	0/1966	0.71	0/2674
1	D	0.58	0/2063	0.74	0/2807
1	E	0.56	0/2076	0.74	0/2826
1	F	0.60	0/1902	0.73	0/2586
1	G	0.57	0/2063	0.75	2/2808 (0.1%)
1	H	0.60	0/2025	0.75	3/2758 (0.1%)
1	I	0.60	0/1937	0.72	0/2631
1	J	0.56	0/2042	0.71	0/2780
1	K	0.62	0/2061	0.79	1/2802 (0.0%)
1	L	0.60	0/1947	0.74	1/2646 (0.0%)
All	All	0.59	0/24212	0.74	10/32941 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	MET	C-N-CA	6.46	137.86	121.70
1	G	371	MET	C-N-CA	6.05	136.82	121.70
1	G	371	MET	CA-C-N	5.46	129.22	117.20
1	A	371	MET	CA-C-N	5.31	128.89	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	340	LEU	CA-CB-CG	5.25	127.37	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	376	SER	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2001	0	1812	20	0
1	B	2037	0	1879	18	0
1	C	1922	0	1761	10	0
1	D	2013	0	1859	22	0
1	E	2028	0	1865	15	0
1	F	1860	0	1699	12	0
1	G	2014	0	1856	13	0
1	H	1982	0	1816	11	0
1	I	1895	0	1736	14	0
1	J	1993	0	1842	15	0
1	K	2016	0	1858	20	0
1	L	1904	0	1744	17	0
2	A	41	0	61	0	0
2	C	20	0	30	0	0
3	A	12	0	16	0	0
3	B	9	0	14	0	0
3	C	9	0	14	0	0
3	I	16	0	31	4	0
All	All	23772	0	21893	177	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 4.

The worst 5 of 177 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:C:170:VAL:HG13	1:C:206:VAL:HG22	1.67	0.75
1:H:203:ILE:O	1:H:260:THR:HG21	1.90	0.71
1:L:150:TRP:HB2	1:L:174:TYR:HB3	1.78	0.66
1:K:163:ARG:NH1	1:K:213:LYS:O	2.31	0.63
1:L:301:SER:O	1:L:303:VAL:N	2.31	0.63

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/334 (78%)	241 (93%)	14 (5%)	5 (2%)	8	31
1	B	264/334 (79%)	243 (92%)	17 (6%)	4 (2%)	10	37
1	C	249/334 (75%)	231 (93%)	16 (6%)	2 (1%)	19	52
1	D	263/334 (79%)	242 (92%)	15 (6%)	6 (2%)	6	26
1	E	265/334 (79%)	237 (89%)	21 (8%)	7 (3%)	5	24
1	F	238/334 (71%)	216 (91%)	17 (7%)	5 (2%)	7	28
1	G	261/334 (78%)	241 (92%)	15 (6%)	5 (2%)	8	31
1	H	262/334 (78%)	237 (90%)	22 (8%)	3 (1%)	14	44
1	I	238/334 (71%)	213 (90%)	22 (9%)	3 (1%)	12	40
1	J	258/334 (77%)	225 (87%)	27 (10%)	6 (2%)	6	26
1	K	260/334 (78%)	238 (92%)	18 (7%)	4 (2%)	10	37
1	L	243/334 (73%)	229 (94%)	12 (5%)	2 (1%)	19	52
All	All	3061/4008 (76%)	2793 (91%)	216 (7%)	52 (2%)	9	34

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	378	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	105	ASN
1	D	161	ASP
1	D	329	GLU
1	E	378	ASN

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	203/280 (72%)	190 (94%)	13 (6%)	17	46
1	B	210/280 (75%)	197 (94%)	13 (6%)	18	48
1	C	194/280 (69%)	184 (95%)	10 (5%)	23	54
1	D	206/280 (74%)	187 (91%)	19 (9%)	9	31
1	E	208/280 (74%)	196 (94%)	12 (6%)	20	50
1	F	186/280 (66%)	170 (91%)	16 (9%)	10	36
1	G	206/280 (74%)	193 (94%)	13 (6%)	18	47
1	H	201/280 (72%)	190 (94%)	11 (6%)	21	52
1	I	193/280 (69%)	182 (94%)	11 (6%)	20	50
1	J	204/280 (73%)	192 (94%)	12 (6%)	19	49
1	K	206/280 (74%)	191 (93%)	15 (7%)	14	42
1	L	193/280 (69%)	181 (94%)	12 (6%)	18	48
All	All	2410/3360 (72%)	2253 (94%)	157 (6%)	17	46

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	334	SER
1	K	378	ASN
1	J	115	THR
1	K	91	SER
1	L	273	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	318	GLN
1	J	304	ASN
1	K	318	GLN
1	I	384	ASN
1	E	318	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	$\# Z > 2$
2	C8E	C	502	-	10,10,20	0.61	0	9,9,19	0.59	0
3	LDA	C	503	-	5,8,15	3.17	1 (20%)	7,10,17	0.53	0
3	LDA	A	504	-	6,9,15	2.93	1 (16%)	8,11,17	0.71	0
2	C8E	A	501	-	20,20,20	0.60	0	19,19,19	0.45	0
3	LDA	B	501	-	5,8,15	3.19	1 (20%)	7,10,17	0.55	0
2	C8E	C	501	-	8,8,20	0.55	0	7,7,19	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	C8E	A	503	-	11,11,20	0.73	0	10,10,19	0.46	0
2	C8E	A	502	-	7,7,20	0.56	0	6,6,19	0.22	0
3	LDA	I	501	-	12,15,15	2.11	1 (8%)	14,17,17	0.95	1 (7%)

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	C8E	C	502	-	-	5/8/8/18	-
3	LDA	C	503	-	-	2/6/6/13	-
3	LDA	A	504	-	-	1/7/7/13	-
2	C8E	A	501	-	-	11/18/18/18	-
3	LDA	B	501	-	-	1/6/6/13	-
2	C8E	C	501	-	-	5/6/6/18	-
2	C8E	A	503	-	-	5/9/9/18	-
2	C8E	A	502	-	-	3/5/5/18	-
3	LDA	I	501	-	-	8/13/13/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	501	LDA	O1-N1	-7.24	1.25	1.42
3	A	504	LDA	O1-N1	-7.13	1.25	1.42
3	B	501	LDA	O1-N1	-7.07	1.25	1.42
3	C	503	LDA	O1-N1	-7.03	1.25	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	501	LDA	CM2-N1-C1	2.29	115.05	110.23

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	503	LDA	N1-C1-C2-C3
3	I	501	LDA	C2-C1-N1-O1

Continued on next page...

Continued from previous page...

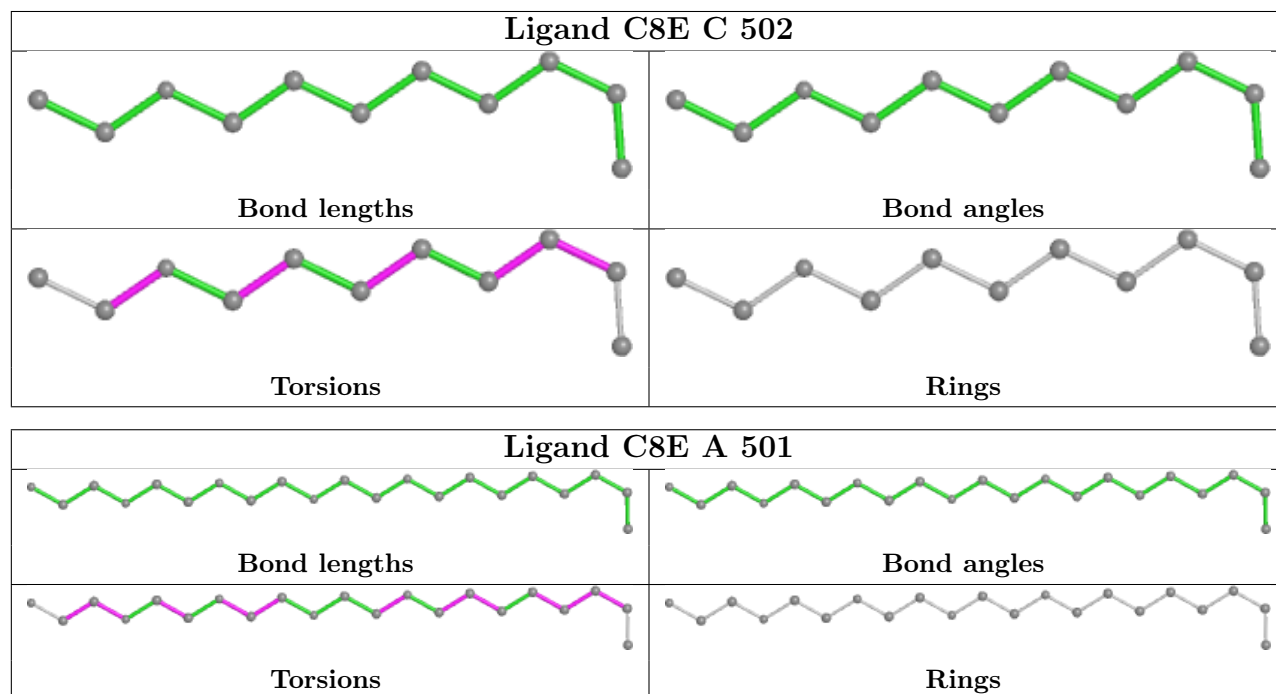
Mol	Chain	Res	Type	Atoms
3	I	501	LDA	C2-C1-N1-CM1
3	I	501	LDA	C2-C1-N1-CM2
2	A	501	C8E	O15-C16-C17-O18

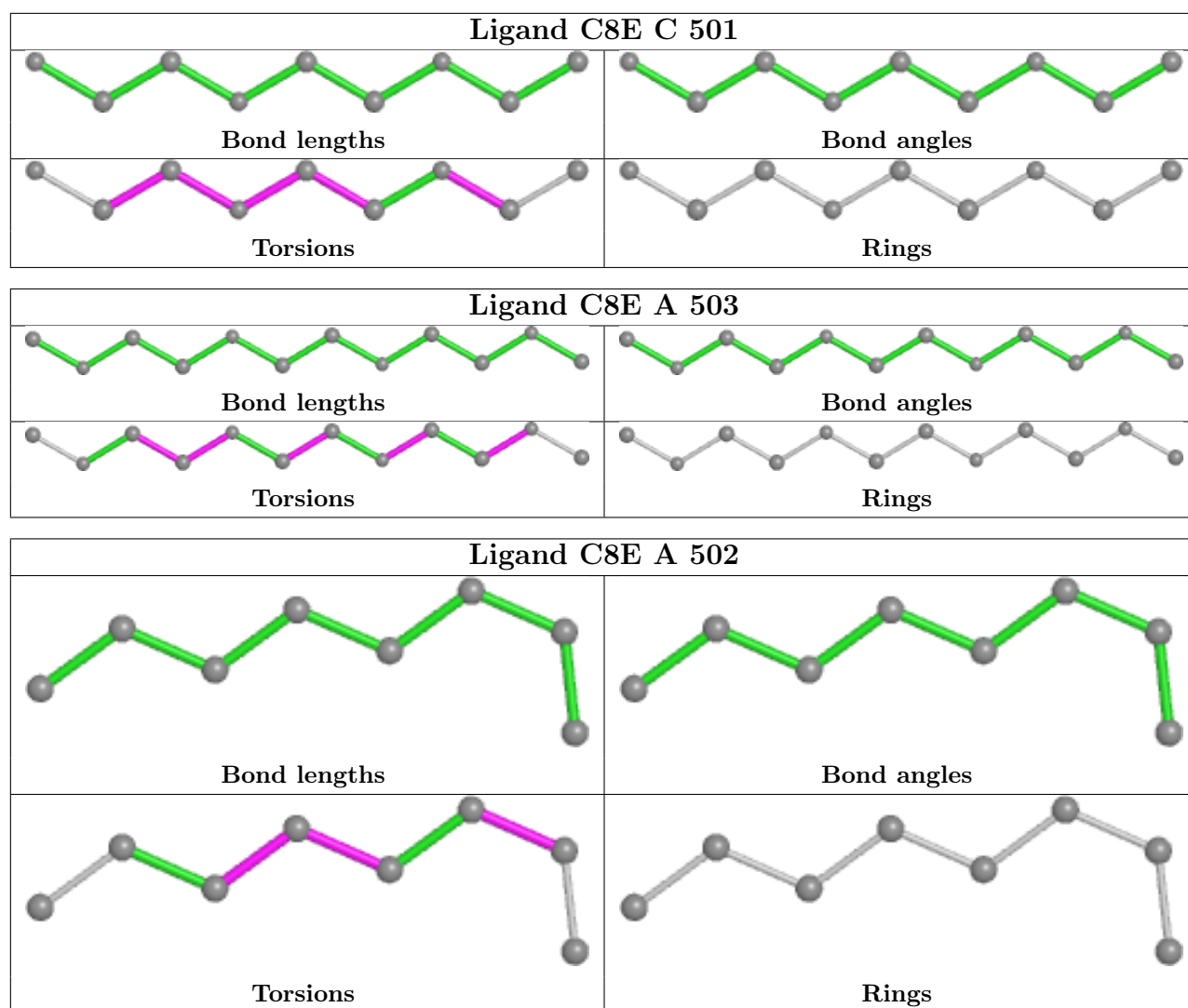
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	501	LDA	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	272/334 (81%)	-0.26	0 100 100	25, 47, 69, 78	0
1	B	274/334 (82%)	-0.03	0 100 100	23, 43, 62, 76	0
1	C	262/334 (78%)	0.19	6 (2%) 60 37	27, 45, 72, 81	0
1	D	271/334 (81%)	-0.24	1 (0%) 92 84	24, 46, 74, 88	0
1	E	273/334 (81%)	-0.02	3 (1%) 80 62	19, 42, 63, 78	0
1	F	254/334 (76%)	0.20	7 (2%) 53 28	24, 45, 68, 78	0
1	G	271/334 (81%)	-0.13	0 100 100	23, 49, 70, 88	0
1	H	272/334 (81%)	-0.11	0 100 100	20, 42, 60, 75	0
1	I	256/334 (76%)	-0.02	0 100 100	22, 46, 68, 83	0
1	J	268/334 (80%)	-0.12	0 100 100	23, 49, 74, 89	0
1	K	272/334 (81%)	-0.06	0 100 100	24, 42, 62, 77	0
1	L	258/334 (77%)	-0.02	1 (0%) 92 84	21, 46, 68, 89	0
All	All	3203/4008 (79%)	-0.05	18 (0%) 89 77	19, 45, 68, 89	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	257	SER	3.1
1	D	392	ASP	3.1
1	C	255	PRO	3.0
1	C	380	THR	2.9
1	C	198	SER	2.8

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

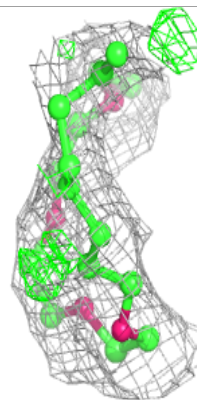
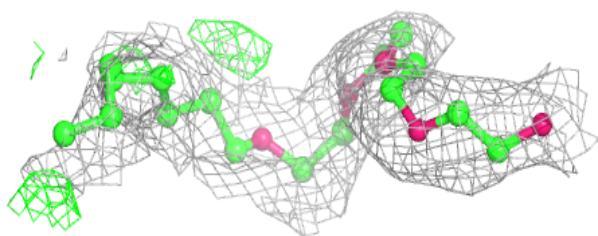
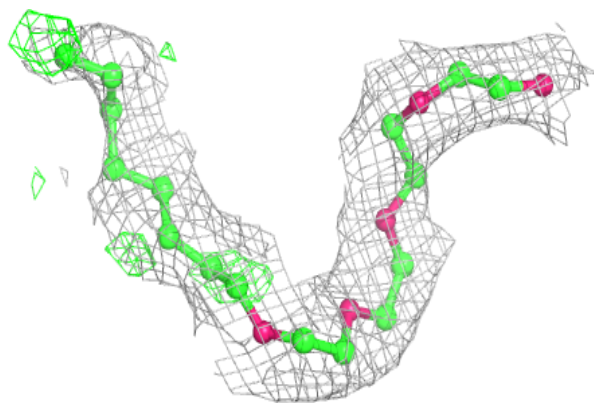
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	LDA	B	501	9/16	0.70	0.30	72,76,80,84	0
2	C8E	A	501	21/21	0.77	0.25	62,80,84,85	0
3	LDA	C	503	9/16	0.82	0.25	74,83,94,96	0
2	C8E	A	502	8/21	0.86	0.40	41,43,44,44	0
2	C8E	C	502	11/21	0.88	0.29	38,39,44,45	0
3	LDA	A	504	12/16	0.88	0.31	7,73,88,89	0
3	LDA	I	501	16/16	0.89	0.28	45,52,61,63	0
2	C8E	A	503	12/21	0.90	0.41	51,56,68,69	0
2	C8E	C	501	9/21	0.91	0.39	64,68,72,72	0

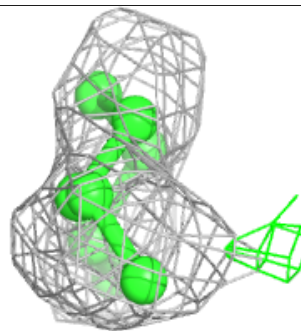
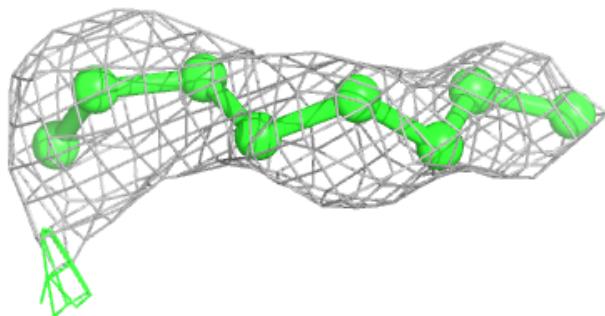
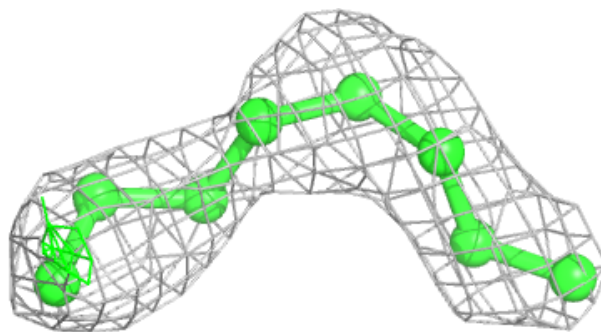
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E 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)

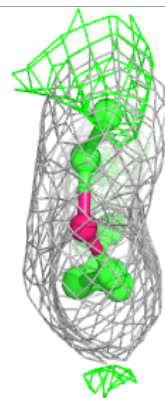
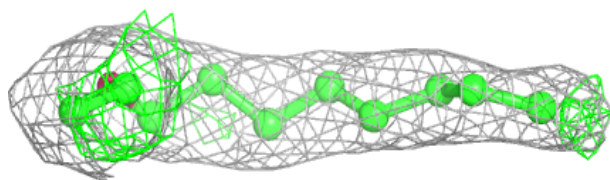
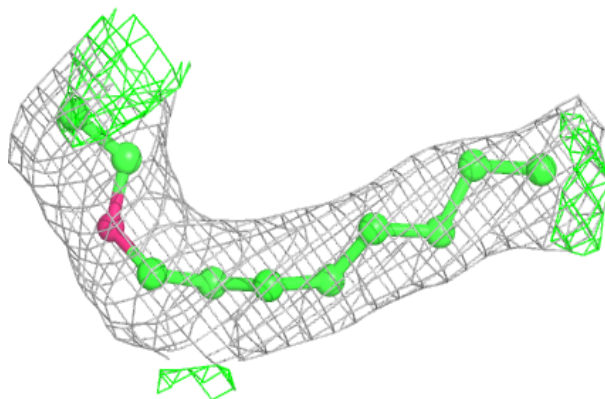
**Electron density around C8E A 502:**

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

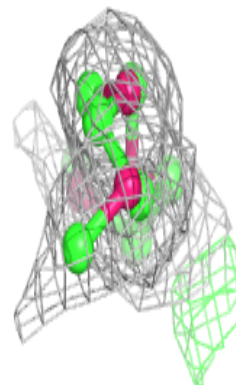
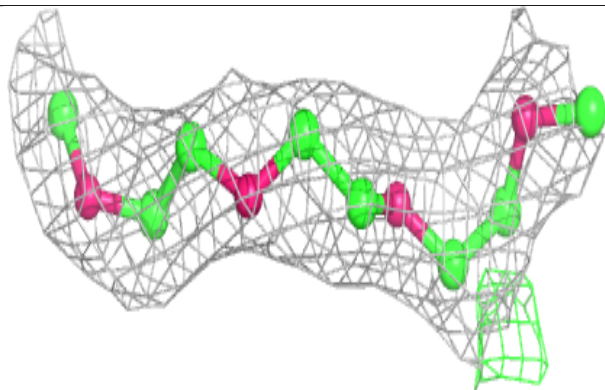
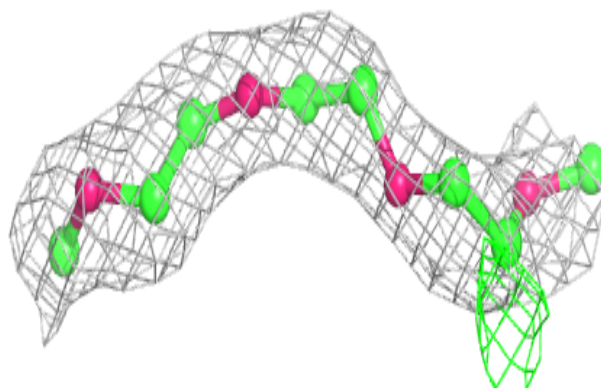


Electron density around C8E C 502:

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

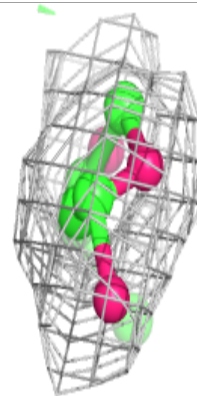
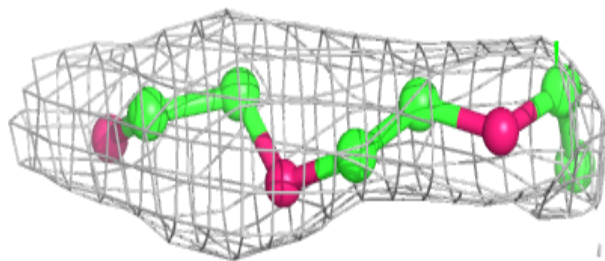
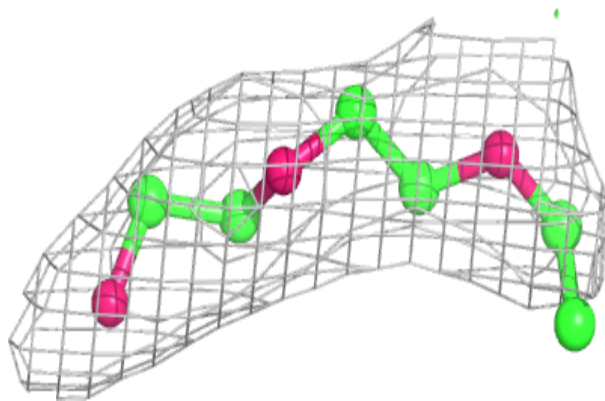
**Electron density around C8E A 503:**

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



Electron density around C8E C 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.