Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:50 pm BST

PDB ID	:	5O67
Title	:	Crystal structure of the FapF polypeptide transporter - F103A 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	:	2.84 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

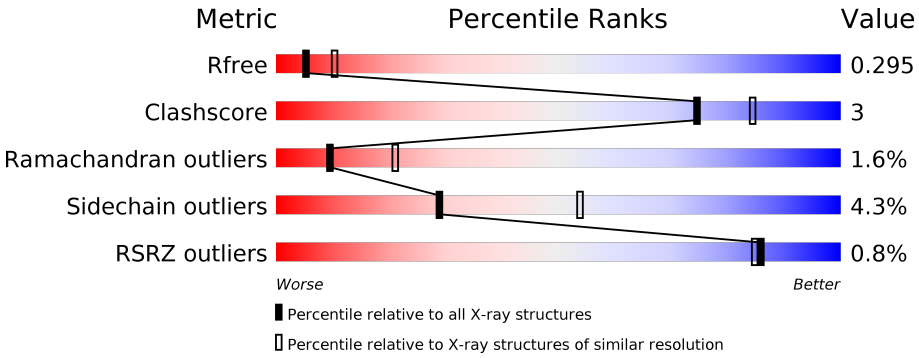
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.84 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	334	% 76% 7% 16%
2	B	334	74% 12% • 13%
2	C	334	% 79% 6% 15%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6629 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	282	Total	C	N	O	S	0	0	0
			2146	1365	349	427	5			

There are 13 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
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	103	ALA	PHE	engineered mutation	UNP C4IN73
A	252	MET	LEU	conflict	UNP C4IN73
A	273	MET	LEU	conflict	UNP C4IN73

- Molecule 2 is a protein called FapF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	291	Total	C	N	O	S	0	0	0
			2212	1408	363	437	4			
2	C	284	Total	C	N	O	S	0	0	0
			2159	1374	354	425	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	73	THR	-	expression tag	UNP C4IN73

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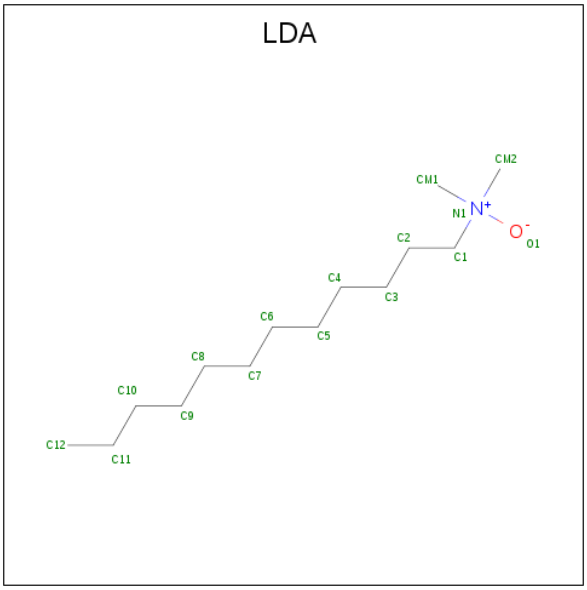
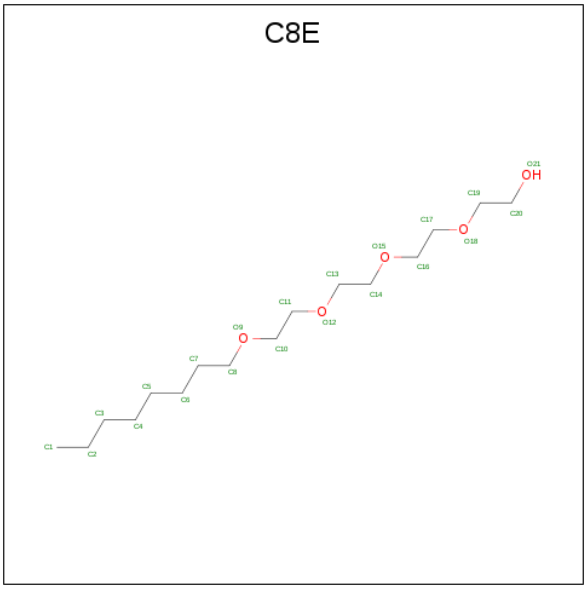
Chain	Residue	Modelled	Actual	Comment	Reference
B	74	SER	-	expression tag	UNP C4IN73
B	75	HIS	-	expression tag	UNP C4IN73
B	76	HIS	-	expression tag	UNP C4IN73
B	77	HIS	-	expression tag	UNP C4IN73
B	78	HIS	-	expression tag	UNP C4IN73
B	79	HIS	-	expression tag	UNP C4IN73
B	80	HIS	-	expression tag	UNP C4IN73
B	81	GLY	-	expression tag	UNP C4IN73
B	82	THR	-	expression tag	UNP C4IN73
B	103	ALA	PHE	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	103	ALA	PHE	engineered mutation	UNP C4IN73
C	273	MET	LEU	conflict	UNP C4IN73

- 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 16 14 1 1	0	0
3	B	1	Total C N O 11 9 1 1	0	0
3	B	1	Total C N O 11 9 1 1	0	0
3	C	1	Total C N O 10 8 1 1	0	0
3	C	1	Total C N O 16 14 1 1	0	0

- Molecule 4 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 14 12 2	0	0
4	C	1	Total C 7 7	0	0
4	C	1	Total C O 14 12 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0

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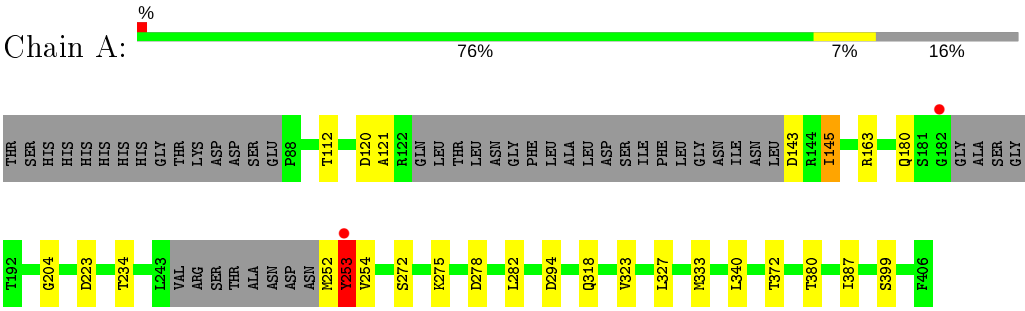
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	9	Total O 9 9	0	0

3 Residue-property plots (i)

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

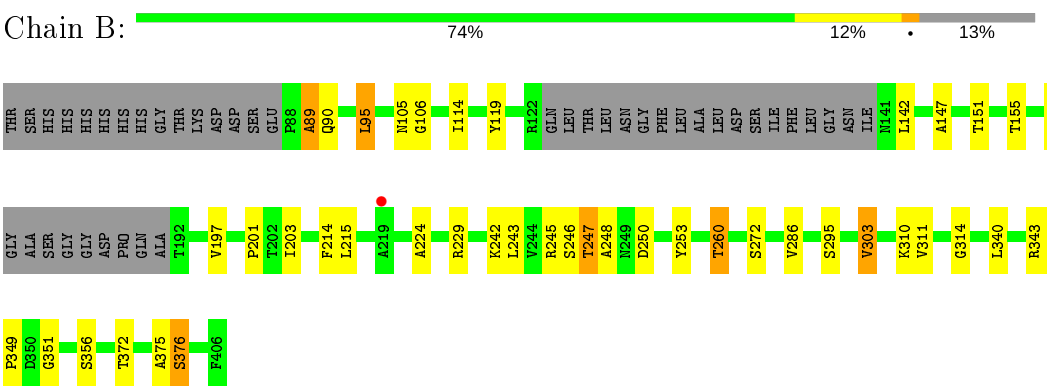
- Molecule 1: FapF

Chain A:



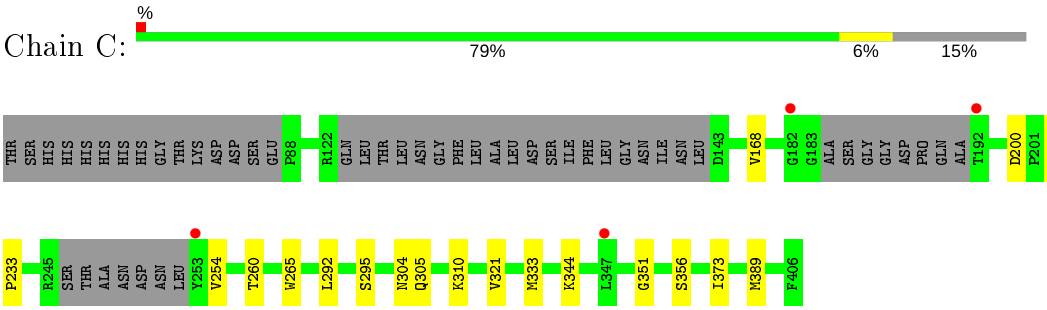
- Molecule 2: FapF

Chain B:



- Molecule 2: FapF

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	147.75Å 125.82Å 81.91Å 90.00° 96.68° 90.00°	Depositor
Resolution (Å)	81.35 – 2.84 81.35 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.8 (81.35-2.84) 99.8 (81.35-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.232 , 0.295 0.237 , 0.295	Depositor DCC
R_{free} test set	1802 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	45.7	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6629	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, C8E

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	0.69	0/2196	0.82	2/2983 (0.1%)
2	B	0.69	0/2263	0.87	1/3076 (0.0%)
2	C	0.64	0/2209	0.78	1/2999 (0.0%)
All	All	0.68	0/6668	0.83	4/9058 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	351	GLY	N-CA-C	-9.11	90.34	113.10
1	A	163	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	253	TYR	C-N-CA	5.40	135.20	121.70
2	C	229	ARG	NE-CZ-NH1	5.34	122.97	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	2146	0	2021	11	0
2	B	2212	0	2096	25	0
2	C	2159	0	2045	6	0
3	A	16	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	22	0	36	0	0
3	C	26	0	47	0	0
4	C	35	0	57	0	0
5	A	4	0	0	0	0
5	C	9	0	0	0	0
All	All	6629	0	6333	41	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 3.

All (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:ALA:HB3	2:B:90:GLN:HA	1.65	0.78
2:B:246:SER:HB2	2:B:247:THR:CB	2.20	0.71
2:B:375:ALA:O	2:B:376:SER:HB3	1.93	0.68
1:A:143:ASP:HB2	1:A:180:GLN:O	1.98	0.64
2:B:89:ALA:CB	2:B:90:GLN:HA	2.29	0.62
2:B:95:LEU:HD12	2:B:95:LEU:O	1.99	0.62
2:B:245:ARG:HD2	2:B:250:ASP:O	2.04	0.58
2:B:311:VAL:HG12	2:B:347:LEU:HD23	1.85	0.57
2:B:242:LYS:HD2	2:B:303:VAL:HA	1.88	0.56
2:C:200:ASP:O	2:C:202:THR:OG1	2.23	0.56
2:B:246:SER:CA	2:B:247:THR:CB	2.84	0.56
2:B:245:ARG:CZ	2:B:245:ARG:HB3	2.36	0.54
2:B:245:ARG:HB3	2:B:245:ARG:NH1	2.22	0.54
2:B:245:ARG:HB2	2:B:253:TYR:CD1	2.43	0.54
2:B:314:GLY:HA3	2:B:343:ARG:O	2.09	0.53
2:B:245:ARG:HB2	2:B:253:TYR:CE1	2.44	0.52
2:B:246:SER:HA	2:B:247:THR:CB	2.40	0.52
2:B:167:ASP:OD2	2:B:229:ARG:NH2	2.44	0.50
2:B:246:SER:CB	2:B:247:THR:CB	2.88	0.50
1:A:252:MET:O	1:A:253:TYR:HB2	2.11	0.49
2:B:114:ILE:HD12	2:B:151:THR:O	2.14	0.47
2:C:265:TRP:HB2	2:C:292:LEU:HD12	1.96	0.47
1:A:282:LEU:HD12	1:A:323:VAL:HG23	1.96	0.47
2:C:265:TRP:CB	2:C:292:LEU:HD12	2.45	0.46
2:B:214:PHE:CE1	2:B:224:ALA:HB1	2.50	0.46
1:A:252:MET:O	1:A:253:TYR:CB	2.64	0.45
2:B:119:TYR:HB2	2:B:147:ALA:HB3	1.98	0.45
2:B:215:LEU:HB2	2:B:224:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:VAL:HG12	2:B:347:LEU:CD2	2.46	0.45
1:A:318:GLN:CG	1:A:340:LEU:HD12	2.48	0.44
2:B:203:ILE:O	2:B:260:THR:HG21	2.18	0.44
1:A:387:ILE:HG12	2:C:389:MET:CE	2.48	0.43
1:A:327:LEU:HD11	1:A:333:MET:HB2	1.99	0.43
1:A:204:GLY:O	1:A:234:THR:OG1	2.35	0.43
2:B:340:LEU:C	2:B:340:LEU:HD23	2.39	0.43
1:A:318:GLN:HG3	1:A:340:LEU:HD12	2.02	0.42
1:A:253:TYR:HB3	1:A:254:VAL:HB	2.02	0.41
2:C:373:ILE:HD12	2:C:373:ILE:N	2.36	0.41
2:C:295:SER:HB3	2:C:310:LYS:HG2	2.03	0.41
2:B:295:SER:HB3	2:B:310:LYS:HG2	2.03	0.40
1:A:121:ALA:HB3	1:A:145:ILE:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	274/334 (82%)	259 (94%)	13 (5%)	2 (1%)	22 42
2	B	285/334 (85%)	269 (94%)	8 (3%)	8 (3%)	5 10
2	C	276/334 (83%)	258 (94%)	15 (5%)	3 (1%)	14 30
All	All	835/1002 (83%)	786 (94%)	36 (4%)	13 (2%)	9 21

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	ILE
1	A	253	TYR
2	B	105	ASN
2	B	106	GLY

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Mol	Chain	Res	Type
2	B	247	THR
2	B	376	SER
2	B	248	ALA
2	B	89	ALA
2	C	305	GLN
2	B	201	PRO
2	C	233	PRO
2	C	351	GLY
2	B	349	PRO

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	230/280 (82%)	220 (96%)	10 (4%)	29 54
2	B	237/280 (85%)	225 (95%)	12 (5%)	24 45
2	C	231/280 (82%)	223 (96%)	8 (4%)	36 61
All	All	698/840 (83%)	668 (96%)	30 (4%)	29 54

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	THR
1	A	120	ASP
1	A	223	ASP
1	A	272	SER
1	A	275	LYS
1	A	278	ASP
1	A	294	ASP
1	A	372	THR
1	A	380	THR
1	A	399	SER
2	B	95	LEU
2	B	142	LEU
2	B	155	THR

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Mol	Chain	Res	Type
2	B	197	VAL
2	B	243	LEU
2	B	260	THR
2	B	272	SER
2	B	286	VAL
2	B	303	VAL
2	B	344	LYS
2	B	356	SER
2	B	372	THR
2	C	168	VAL
2	C	254	VAL
2	C	260	THR
2	C	304	ASN
2	C	321	VAL
2	C	333	MET
2	C	344	LYS
2	C	356	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	162	ASN
1	A	180	GLN
1	A	318	GLN
2	B	149	ASN
2	B	318	GLN
2	B	378	ASN
2	C	105	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
3	LDA	B	502	-	7,10,15	2.66	1 (14%)	9,12,17	0.85	1 (11%)
4	C8E	C	504	-	6,6,20	0.54	0	5,5,19	0.49	0
3	LDA	C	501	-	6,9,15	3.07	1 (16%)	8,11,17	1.26	1 (12%)
3	LDA	A	501	-	12,15,15	2.07	1 (8%)	14,17,17	0.58	0
4	C8E	C	505	-	12,12,20	0.57	0	10,10,19	0.57	0
3	LDA	B	501	-	7,10,15	2.87	1 (14%)	9,12,17	1.30	2 (22%)
3	LDA	C	502	-	12,15,15	2.12	1 (8%)	14,17,17	0.50	0
4	C8E	C	503	-	13,13,20	0.66	0	12,12,19	0.75	0

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
3	LDA	B	502	-	-	7/8/8/13	-
4	C8E	C	504	-	-	3/4/4/18	-
3	LDA	C	501	-	-	7/7/7/13	-
3	LDA	A	501	-	-	5/13/13/13	-
4	C8E	C	505	-	-	5/8/8/18	-
3	LDA	B	501	-	-	4/8/8/13	-
3	LDA	C	502	-	-	6/13/13/13	-
4	C8E	C	503	-	-	4/11/11/18	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	LDA	O1-N1	-7.49	1.24	1.42
3	C	501	LDA	O1-N1	-7.38	1.24	1.42
3	C	502	LDA	O1-N1	-7.19	1.25	1.42
3	A	501	LDA	O1-N1	-7.00	1.25	1.42
3	B	502	LDA	O1-N1	-6.92	1.26	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	LDA	CM1-N1-C1	3.14	116.83	110.23
3	C	501	LDA	CM2-N1-C1	2.94	116.41	110.23
3	B	501	LDA	O1-N1-C1	-2.16	103.97	109.27
3	B	502	LDA	CM2-N1-C1	2.09	114.62	110.23

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	LDA	C2-C1-N1-O1
3	B	502	LDA	C2-C1-N1-CM2
3	C	501	LDA	C2-C1-N1-CM1
3	C	501	LDA	C2-C1-N1-CM2
3	C	501	LDA	N1-C1-C2-C3
3	A	501	LDA	N1-C1-C2-C3
3	C	502	LDA	C7-C8-C9-C10
3	C	502	LDA	C3-C4-C5-C6
4	C	503	C8E	C4-C5-C6-C7
3	C	502	LDA	C6-C7-C8-C9
3	C	501	LDA	C2-C3-C4-C5
4	C	503	C8E	O9-C10-C11-O12
3	B	502	LDA	C3-C4-C5-C6
3	A	501	LDA	C2-C3-C4-C5
3	A	501	LDA	C5-C6-C7-C8
3	B	501	LDA	C3-C4-C5-C6
3	B	501	LDA	C2-C3-C4-C5
4	C	504	C8E	C2-C3-C4-C5
4	C	505	C8E	C3-C4-C5-C6
4	C	505	C8E	O15-C16-C17-O18
3	C	502	LDA	C1-C2-C3-C4
3	C	502	LDA	C11-C10-C9-C8
3	B	502	LDA	C1-C2-C3-C4

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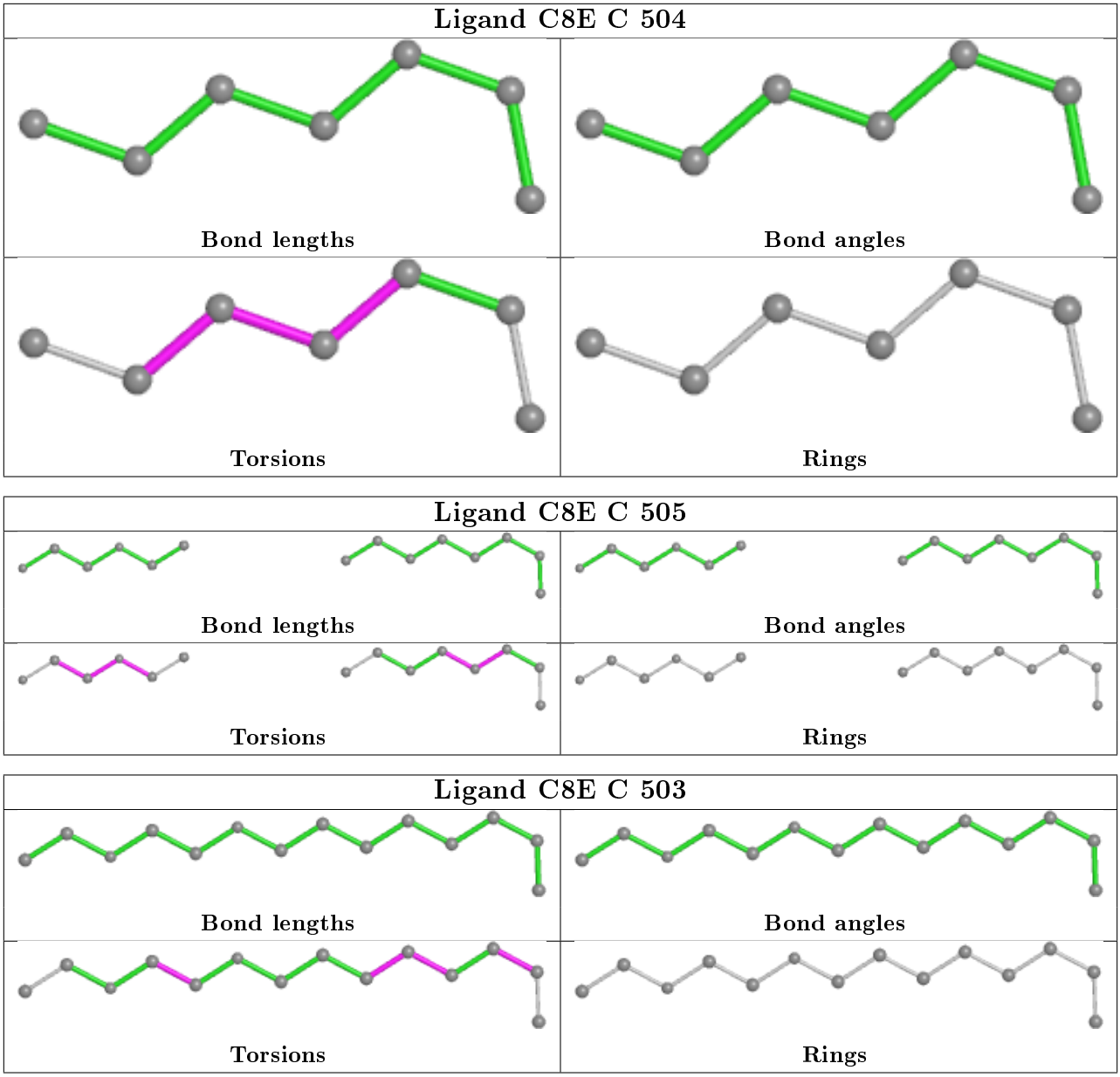
Mol	Chain	Res	Type	Atoms
3	A	501	LDA	C4-C5-C6-C7
4	C	504	C8E	C3-C4-C5-C6
4	C	503	C8E	C1-C2-C3-C4
3	A	501	LDA	C1-C2-C3-C4
3	B	502	LDA	N1-C1-C2-C3
3	B	501	LDA	N1-C1-C2-C3
3	C	501	LDA	C1-C2-C3-C4
3	B	502	LDA	C2-C3-C4-C5
3	B	501	LDA	C4-C5-C6-C7
3	B	502	LDA	C2-C1-N1-CM1
3	C	501	LDA	C3-C4-C5-C6
4	C	503	C8E	C3-C4-C5-C6
4	C	505	C8E	C13-C14-O15-C16
4	C	505	C8E	C2-C3-C4-C5
4	C	505	C8E	C17-C16-O15-C14
3	C	502	LDA	C4-C5-C6-C7
4	C	504	C8E	C4-C5-C6-C7
3	C	501	LDA	C2-C1-N1-O1

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 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.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	282/334 (84%)	-0.05	2 (0%)	87	86	21, 44, 73, 113	0
2	B	291/334 (87%)	-0.11	1 (0%)	94	93	23, 41, 70, 103	0
2	C	284/334 (85%)	-0.02	4 (1%)	75	71	23, 44, 81, 95	0
All	All	857/1002 (85%)	-0.06	7 (0%)	86	85	21, 43, 77, 113	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	TYR	4.5
1	A	182	GLY	2.9
2	C	253	TYR	2.5
2	C	182	GLY	2.2
2	C	192	THR	2.1
2	C	347	LEU	2.1
2	B	219	ALA	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

There are no carbohydrates 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,

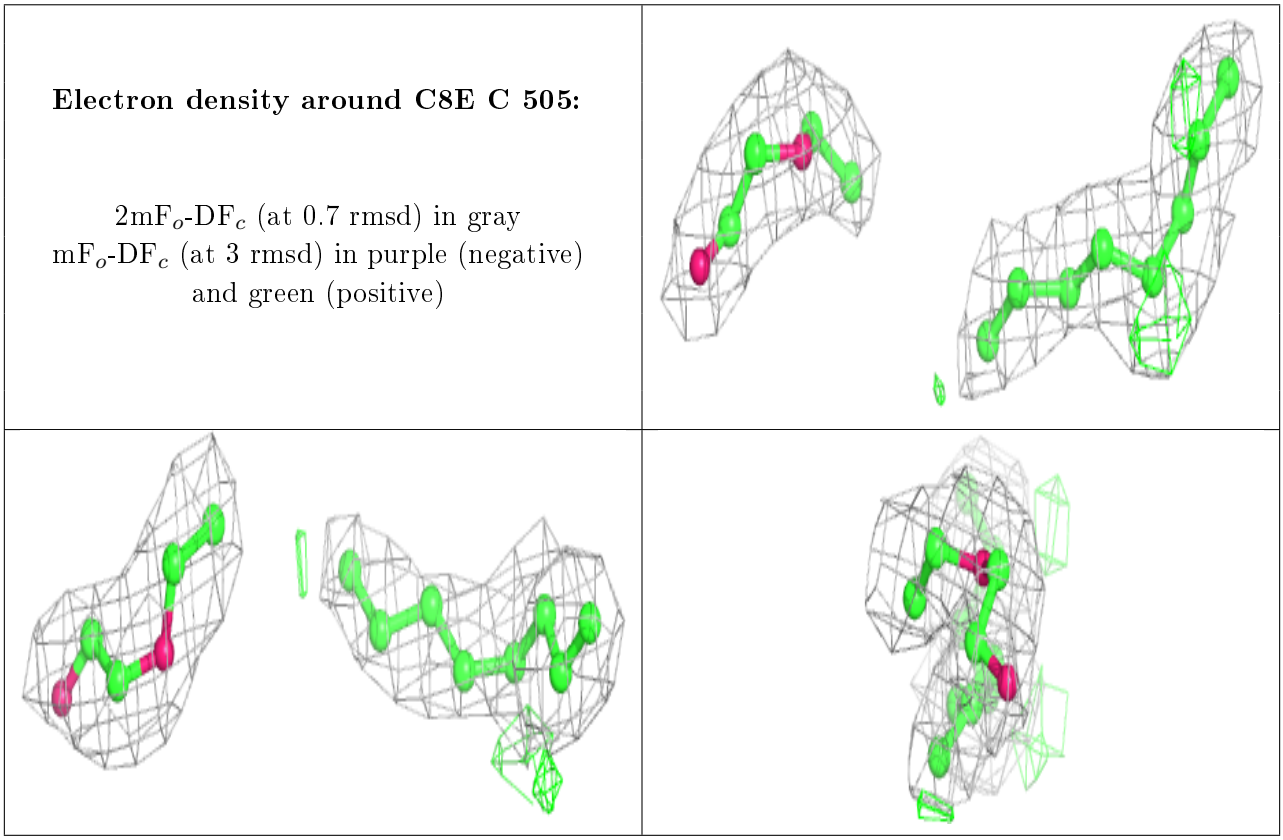
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LDA	B	501	11/16	0.69	0.27	73,84,94,96	0
3	LDA	C	501	10/16	0.70	0.26	78,86,95,95	0
3	LDA	A	501	16/16	0.71	0.26	93,104,112,118	0
3	LDA	B	502	11/16	0.79	0.27	61,70,94,97	0
3	LDA	C	502	16/16	0.81	0.30	55,64,108,110	0
4	C8E	C	505	14/21	0.90	0.21	34,52,65,66	0
4	C8E	C	503	14/21	0.90	0.21	51,56,59,61	0
4	C8E	C	504	7/21	0.92	0.24	45,49,56,56	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.

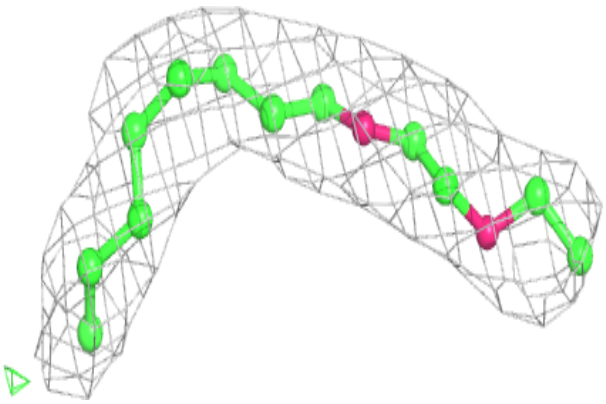
Electron density around C8E C 505:

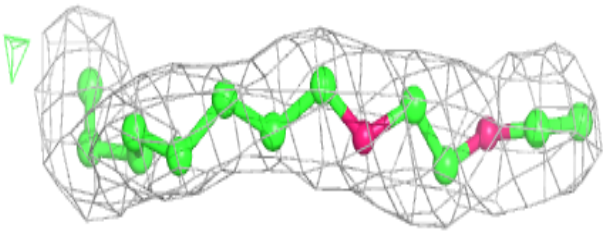
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

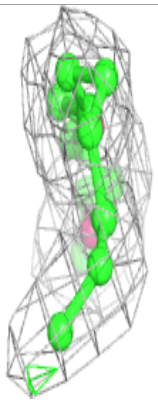


Electron density around C8E C 503:

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

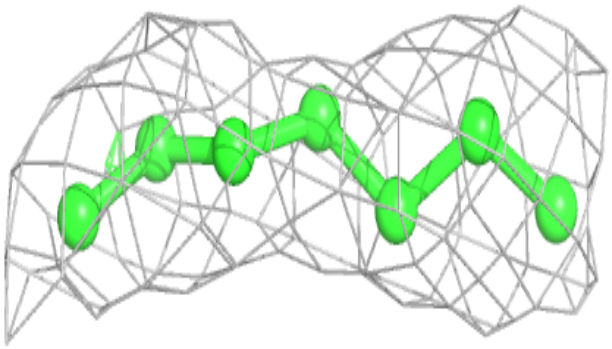


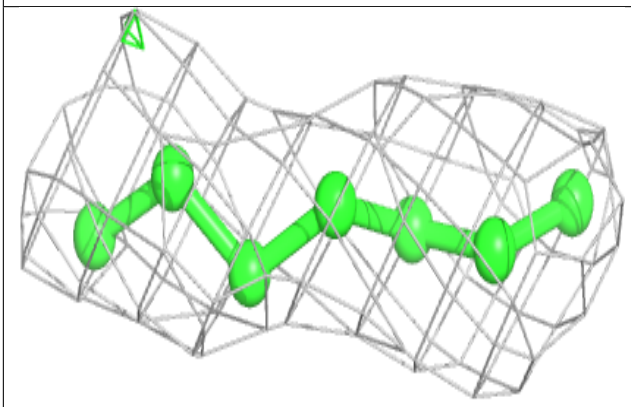


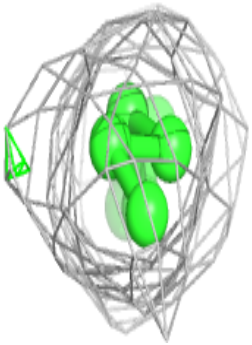


Electron density around C8E C 504:

$2mF_o$-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.