Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 05:55 PM JST

PDB ID	:	6LUA
Title	:	Cis-mutant R349A of the central AAA+ domain of the flagellar regulatory protein FlrC
Authors	:	Dasgupta, J.; Chakraborty, S.
Deposited on	:	2020-01-27
Resolution	:	3.10 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

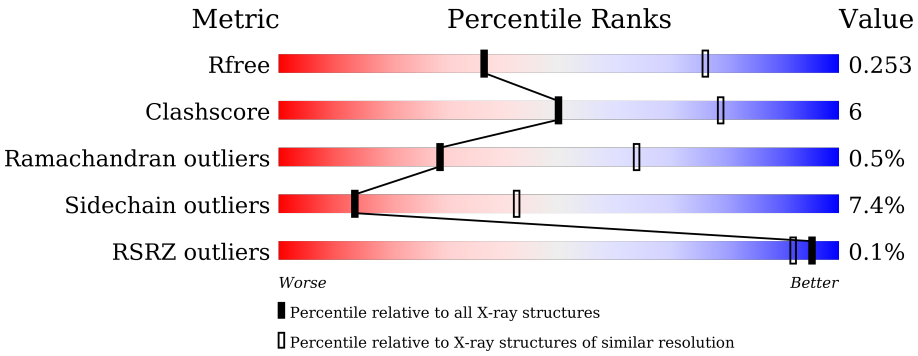
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	271	75% 15% • 9%
1	B	271	70% 18% • 9%
1	C	271	79% 11% • 9%
1	D	271	70% 19% • 9%
1	E	271	74% 15% • 9%
1	F	271	74% 16% • 9%

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Mol	Chain	Length	Quality of chain
1	G	271	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13507 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 Flagellar regulatory protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1924	1220	340	355	9			
1	B	247	Total	C	N	O	S	0	0	0
			1924	1220	340	355	9			
1	C	247	Total	C	N	O	S	0	1	0
			1932	1225	343	355	9			
1	D	246	Total	C	N	O	S	0	0	0
			1914	1214	337	354	9			
1	E	246	Total	C	N	O	S	0	0	0
			1914	1214	337	354	9			
1	F	247	Total	C	N	O	S	0	0	0
			1924	1220	340	355	9			
1	G	246	Total	C	N	O	S	0	0	0
			1914	1214	337	354	9			

There are 154 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	MET	-	initiating methionine	UNP A0A0H3AHP1
A	112	GLY	-	expression tag	UNP A0A0H3AHP1
A	113	SER	-	expression tag	UNP A0A0H3AHP1
A	114	SER	-	expression tag	UNP A0A0H3AHP1
A	115	HIS	-	expression tag	UNP A0A0H3AHP1
A	116	HIS	-	expression tag	UNP A0A0H3AHP1
A	117	HIS	-	expression tag	UNP A0A0H3AHP1
A	118	HIS	-	expression tag	UNP A0A0H3AHP1
A	119	HIS	-	expression tag	UNP A0A0H3AHP1
A	120	HIS	-	expression tag	UNP A0A0H3AHP1
A	121	SER	-	expression tag	UNP A0A0H3AHP1
A	122	SER	-	expression tag	UNP A0A0H3AHP1
A	123	GLY	-	expression tag	UNP A0A0H3AHP1
A	124	LEU	-	expression tag	UNP A0A0H3AHP1
A	125	VAL	-	expression tag	UNP A0A0H3AHP1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	126	PRO	-	expression tag	UNP A0A0H3AHP1
A	127	ARG	-	expression tag	UNP A0A0H3AHP1
A	128	GLY	-	expression tag	UNP A0A0H3AHP1
A	129	SER	-	expression tag	UNP A0A0H3AHP1
A	130	HIS	-	expression tag	UNP A0A0H3AHP1
A	131	MET	-	expression tag	UNP A0A0H3AHP1
A	349	ALA	ARG	engineered mutation	UNP A0A0H3AHP1
B	111	MET	-	initiating methionine	UNP A0A0H3AHP1
B	112	GLY	-	expression tag	UNP A0A0H3AHP1
B	113	SER	-	expression tag	UNP A0A0H3AHP1
B	114	SER	-	expression tag	UNP A0A0H3AHP1
B	115	HIS	-	expression tag	UNP A0A0H3AHP1
B	116	HIS	-	expression tag	UNP A0A0H3AHP1
B	117	HIS	-	expression tag	UNP A0A0H3AHP1
B	118	HIS	-	expression tag	UNP A0A0H3AHP1
B	119	HIS	-	expression tag	UNP A0A0H3AHP1
B	120	HIS	-	expression tag	UNP A0A0H3AHP1
B	121	SER	-	expression tag	UNP A0A0H3AHP1
B	122	SER	-	expression tag	UNP A0A0H3AHP1
B	123	GLY	-	expression tag	UNP A0A0H3AHP1
B	124	LEU	-	expression tag	UNP A0A0H3AHP1
B	125	VAL	-	expression tag	UNP A0A0H3AHP1
B	126	PRO	-	expression tag	UNP A0A0H3AHP1
B	127	ARG	-	expression tag	UNP A0A0H3AHP1
B	128	GLY	-	expression tag	UNP A0A0H3AHP1
B	129	SER	-	expression tag	UNP A0A0H3AHP1
B	130	HIS	-	expression tag	UNP A0A0H3AHP1
B	131	MET	-	expression tag	UNP A0A0H3AHP1
B	349	ALA	ARG	engineered mutation	UNP A0A0H3AHP1
C	111	MET	-	initiating methionine	UNP A0A0H3AHP1
C	112	GLY	-	expression tag	UNP A0A0H3AHP1
C	113	SER	-	expression tag	UNP A0A0H3AHP1
C	114	SER	-	expression tag	UNP A0A0H3AHP1
C	115	HIS	-	expression tag	UNP A0A0H3AHP1
C	116	HIS	-	expression tag	UNP A0A0H3AHP1
C	117	HIS	-	expression tag	UNP A0A0H3AHP1
C	118	HIS	-	expression tag	UNP A0A0H3AHP1
C	119	HIS	-	expression tag	UNP A0A0H3AHP1
C	120	HIS	-	expression tag	UNP A0A0H3AHP1
C	121	SER	-	expression tag	UNP A0A0H3AHP1
C	122	SER	-	expression tag	UNP A0A0H3AHP1
C	123	GLY	-	expression tag	UNP A0A0H3AHP1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	124	LEU	-	expression tag	UNP A0A0H3AHP1
C	125	VAL	-	expression tag	UNP A0A0H3AHP1
C	126	PRO	-	expression tag	UNP A0A0H3AHP1
C	127	ARG	-	expression tag	UNP A0A0H3AHP1
C	128	GLY	-	expression tag	UNP A0A0H3AHP1
C	129	SER	-	expression tag	UNP A0A0H3AHP1
C	130	HIS	-	expression tag	UNP A0A0H3AHP1
C	131	MET	-	expression tag	UNP A0A0H3AHP1
C	349	ALA	ARG	engineered mutation	UNP A0A0H3AHP1
D	111	MET	-	initiating methionine	UNP A0A0H3AHP1
D	112	GLY	-	expression tag	UNP A0A0H3AHP1
D	113	SER	-	expression tag	UNP A0A0H3AHP1
D	114	SER	-	expression tag	UNP A0A0H3AHP1
D	115	HIS	-	expression tag	UNP A0A0H3AHP1
D	116	HIS	-	expression tag	UNP A0A0H3AHP1
D	117	HIS	-	expression tag	UNP A0A0H3AHP1
D	118	HIS	-	expression tag	UNP A0A0H3AHP1
D	119	HIS	-	expression tag	UNP A0A0H3AHP1
D	120	HIS	-	expression tag	UNP A0A0H3AHP1
D	121	SER	-	expression tag	UNP A0A0H3AHP1
D	122	SER	-	expression tag	UNP A0A0H3AHP1
D	123	GLY	-	expression tag	UNP A0A0H3AHP1
D	124	LEU	-	expression tag	UNP A0A0H3AHP1
D	125	VAL	-	expression tag	UNP A0A0H3AHP1
D	126	PRO	-	expression tag	UNP A0A0H3AHP1
D	127	ARG	-	expression tag	UNP A0A0H3AHP1
D	128	GLY	-	expression tag	UNP A0A0H3AHP1
D	129	SER	-	expression tag	UNP A0A0H3AHP1
D	130	HIS	-	expression tag	UNP A0A0H3AHP1
D	131	MET	-	expression tag	UNP A0A0H3AHP1
D	349	ALA	ARG	engineered mutation	UNP A0A0H3AHP1
E	111	MET	-	initiating methionine	UNP A0A0H3AHP1
E	112	GLY	-	expression tag	UNP A0A0H3AHP1
E	113	SER	-	expression tag	UNP A0A0H3AHP1
E	114	SER	-	expression tag	UNP A0A0H3AHP1
E	115	HIS	-	expression tag	UNP A0A0H3AHP1
E	116	HIS	-	expression tag	UNP A0A0H3AHP1
E	117	HIS	-	expression tag	UNP A0A0H3AHP1
E	118	HIS	-	expression tag	UNP A0A0H3AHP1
E	119	HIS	-	expression tag	UNP A0A0H3AHP1
E	120	HIS	-	expression tag	UNP A0A0H3AHP1
E	121	SER	-	expression tag	UNP A0A0H3AHP1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	122	SER	-	expression tag	UNP A0A0H3AHP1
E	123	GLY	-	expression tag	UNP A0A0H3AHP1
E	124	LEU	-	expression tag	UNP A0A0H3AHP1
E	125	VAL	-	expression tag	UNP A0A0H3AHP1
E	126	PRO	-	expression tag	UNP A0A0H3AHP1
E	127	ARG	-	expression tag	UNP A0A0H3AHP1
E	128	GLY	-	expression tag	UNP A0A0H3AHP1
E	129	SER	-	expression tag	UNP A0A0H3AHP1
E	130	HIS	-	expression tag	UNP A0A0H3AHP1
E	131	MET	-	expression tag	UNP A0A0H3AHP1
E	349	ALA	ARG	engineered mutation	UNP A0A0H3AHP1
F	111	MET	-	initiating methionine	UNP A0A0H3AHP1
F	112	GLY	-	expression tag	UNP A0A0H3AHP1
F	113	SER	-	expression tag	UNP A0A0H3AHP1
F	114	SER	-	expression tag	UNP A0A0H3AHP1
F	115	HIS	-	expression tag	UNP A0A0H3AHP1
F	116	HIS	-	expression tag	UNP A0A0H3AHP1
F	117	HIS	-	expression tag	UNP A0A0H3AHP1
F	118	HIS	-	expression tag	UNP A0A0H3AHP1
F	119	HIS	-	expression tag	UNP A0A0H3AHP1
F	120	HIS	-	expression tag	UNP A0A0H3AHP1
F	121	SER	-	expression tag	UNP A0A0H3AHP1
F	122	SER	-	expression tag	UNP A0A0H3AHP1
F	123	GLY	-	expression tag	UNP A0A0H3AHP1
F	124	LEU	-	expression tag	UNP A0A0H3AHP1
F	125	VAL	-	expression tag	UNP A0A0H3AHP1
F	126	PRO	-	expression tag	UNP A0A0H3AHP1
F	127	ARG	-	expression tag	UNP A0A0H3AHP1
F	128	GLY	-	expression tag	UNP A0A0H3AHP1
F	129	SER	-	expression tag	UNP A0A0H3AHP1
F	130	HIS	-	expression tag	UNP A0A0H3AHP1
F	131	MET	-	expression tag	UNP A0A0H3AHP1
F	349	ALA	ARG	engineered mutation	UNP A0A0H3AHP1
G	111	MET	-	initiating methionine	UNP A0A0H3AHP1
G	112	GLY	-	expression tag	UNP A0A0H3AHP1
G	113	SER	-	expression tag	UNP A0A0H3AHP1
G	114	SER	-	expression tag	UNP A0A0H3AHP1
G	115	HIS	-	expression tag	UNP A0A0H3AHP1
G	116	HIS	-	expression tag	UNP A0A0H3AHP1
G	117	HIS	-	expression tag	UNP A0A0H3AHP1
G	118	HIS	-	expression tag	UNP A0A0H3AHP1
G	119	HIS	-	expression tag	UNP A0A0H3AHP1

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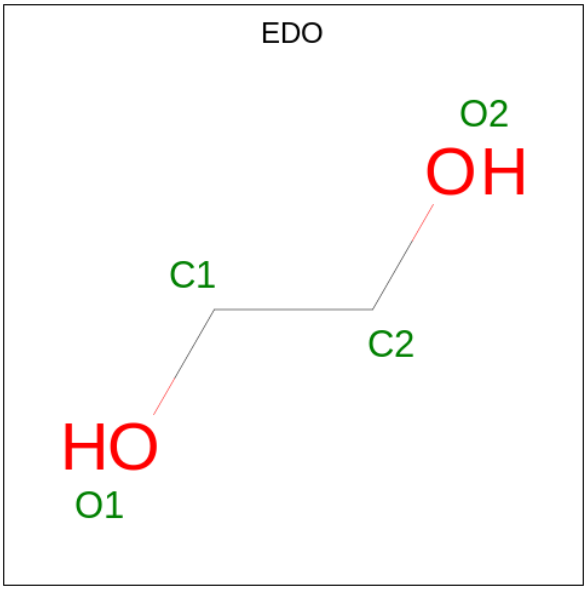
Chain	Residue	Modelled	Actual	Comment	Reference
G	120	HIS	-	expression tag	UNP A0A0H3AHP1
G	121	SER	-	expression tag	UNP A0A0H3AHP1
G	122	SER	-	expression tag	UNP A0A0H3AHP1
G	123	GLY	-	expression tag	UNP A0A0H3AHP1
G	124	LEU	-	expression tag	UNP A0A0H3AHP1
G	125	VAL	-	expression tag	UNP A0A0H3AHP1
G	126	PRO	-	expression tag	UNP A0A0H3AHP1
G	127	ARG	-	expression tag	UNP A0A0H3AHP1
G	128	GLY	-	expression tag	UNP A0A0H3AHP1
G	129	SER	-	expression tag	UNP A0A0H3AHP1
G	130	HIS	-	expression tag	UNP A0A0H3AHP1
G	131	MET	-	expression tag	UNP A0A0H3AHP1
G	349	ALA	ARG	engineered mutation	UNP A0A0H3AHP1

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

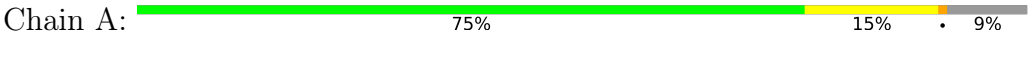
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0
3	B	3	Total O 3 3	0	0
3	C	3	Total O 3 3	0	0
3	D	5	Total O 5 5	0	0
3	E	6	Total O 6 6	0	0
3	F	6	Total O 6 6	0	0
3	G	6	Total O 6 6	0	0

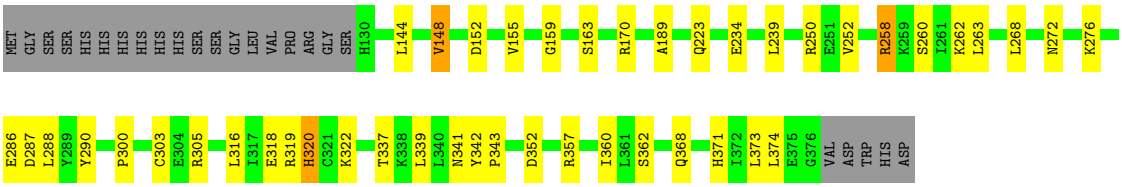
3 Residue-property plots (i)

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: Flagellar regulatory protein C

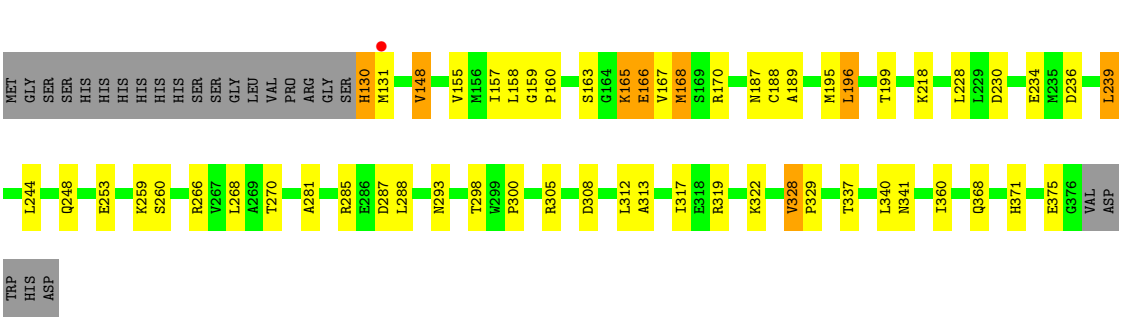
Chain A:





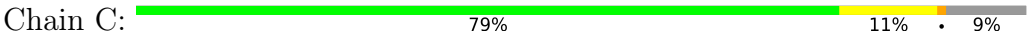
• Molecule 1: Flagellar regulatory protein C

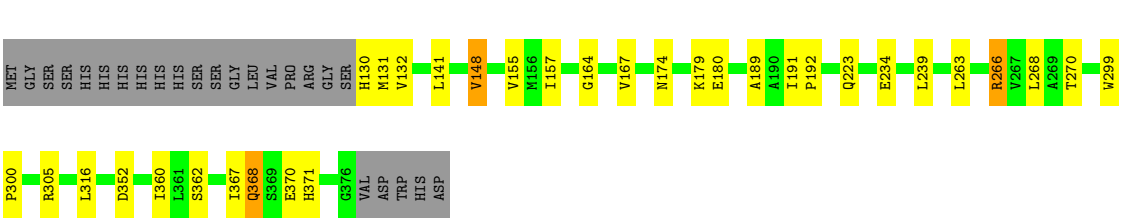
Chain B:



• Molecule 1: Flagellar regulatory protein C

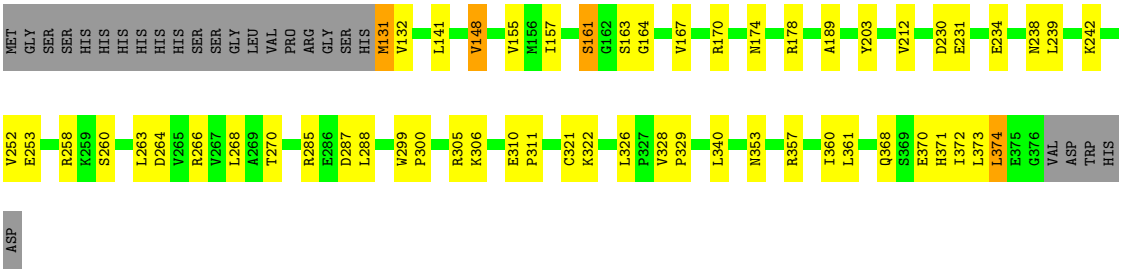
Chain C:





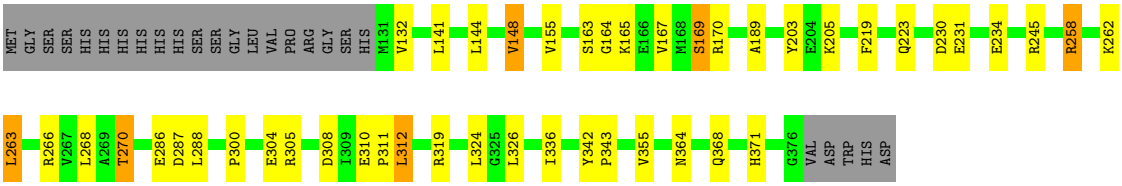
• Molecule 1: Flagellar regulatory protein C

Chain D:



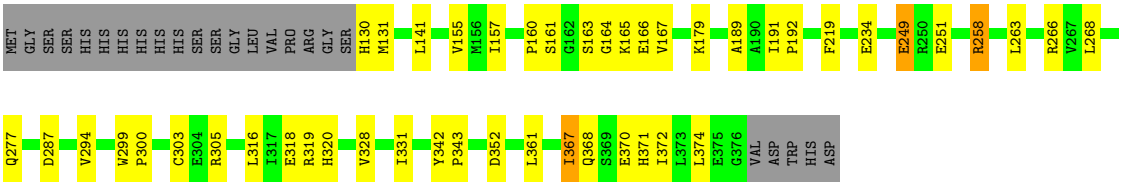
• Molecule 1: Flagellar regulatory protein C

Chain E:



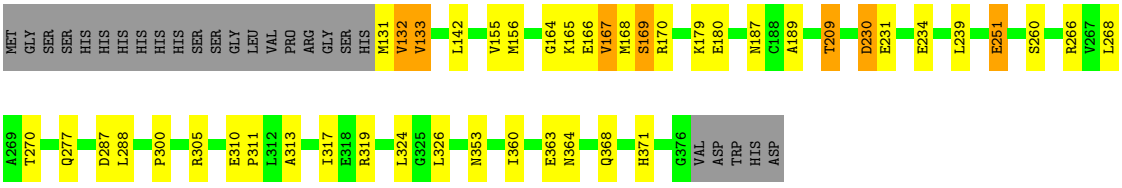
• Molecule 1: Flagellar regulatory protein C

Chain F:



• Molecule 1: Flagellar regulatory protein C

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	80.75Å 154.63Å 194.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 3.10 48.65 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.65-3.10) 93.1 (48.65-3.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.190 , 0.251 0.199 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 20.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13507	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: EDO

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	0.28	0/1959	0.39	0/2652
1	B	0.51	0/1959	0.50	2/2652 (0.1%)
1	C	0.23	0/1970	0.38	0/2666
1	D	0.31	0/1948	0.42	0/2637
1	E	0.29	0/1948	0.39	0/2637
1	F	0.32	0/1959	0.39	0/2652
1	G	0.22	0/1948	0.38	0/2637
All	All	0.32	0/13691	0.41	2/18533 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	159	GLY	C-N-CD	6.58	142.21	128.40
1	B	160	PRO	CA-N-CD	-5.23	104.18	111.50

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	1924	0	1966	25	0
1	B	1924	0	1966	28	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1932	0	1979	17	0
1	D	1914	0	1959	30	0
1	E	1914	0	1959	25	1
1	F	1924	0	1966	24	0
1	G	1914	0	1959	20	0
2	A	4	0	6	1	0
2	B	4	0	6	1	0
2	C	4	0	6	0	0
2	D	4	0	6	1	0
2	E	4	0	6	1	0
2	F	4	0	6	0	0
2	G	4	0	6	0	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	5	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
All	All	13507	0	13796	158	1

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 6.

All (158) 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:D:203:TYR:OH	1:E:258:ARG:NH1	1.70	1.23
1:B:195:MET:O	1:B:199:THR:HG23	1.42	1.17
1:D:212:VAL:HG12	1:E:258:ARG:NH2	1.85	0.90
1:B:165:LYS:O	1:B:168:MET:N	2.11	0.83
1:B:165:LYS:O	1:B:167:VAL:N	2.11	0.82
1:E:286:GLU:HB3	2:E:401:EDO:H21	1.67	0.76
1:D:212:VAL:HG12	1:E:258:ARG:HH21	1.47	0.75
1:F:219:PHE:HB3	1:F:263:LEU:HD21	1.74	0.70
1:A:258:ARG:H	1:A:258:ARG:HD2	1.57	0.69
1:A:337:THR:O	1:A:341:ASN:ND2	2.26	0.69
1:E:165:LYS:O	1:E:169:SER:OG	2.12	0.68
1:G:368:GLN:H	1:G:371:HIS:HD2	1.41	0.68
1:C:189:ALA:HB2	1:C:234:GLU:HG3	1.75	0.67
1:A:189:ALA:HB2	1:A:234:GLU:HG3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:GLU:HB3	1:F:251:GLU:HG2	1.76	0.67
1:B:166:GLU:O	1:B:166:GLU:HG2	1.94	0.66
1:E:219:PHE:HB3	1:E:263:LEU:HD21	1.78	0.66
1:B:195:MET:O	1:B:199:THR:CG2	2.34	0.66
1:D:203:TYR:CZ	1:E:258:ARG:NH1	2.62	0.65
1:B:189:ALA:HB2	1:B:234:GLU:HG3	1.80	0.64
1:F:141:LEU:HD23	1:F:299:TRP:HE3	1.64	0.63
1:D:306:LYS:NZ	1:D:340:LEU:O	2.32	0.62
1:E:189:ALA:HB2	1:E:234:GLU:HG3	1.82	0.62
1:D:141:LEU:HD23	1:D:299:TRP:HE3	1.64	0.62
1:E:300:PRO:HB2	1:E:304:GLU:HG3	1.83	0.61
1:B:300:PRO:HG2	1:B:305:ARG:HD3	1.81	0.61
1:E:231:GLU:H	1:E:270:THR:HG22	1.66	0.60
1:E:155:VAL:HB	1:E:268:LEU:HD22	1.83	0.60
1:D:368:GLN:H	1:D:371:HIS:HD2	1.50	0.59
1:E:368:GLN:H	1:E:371:HIS:CD2	2.20	0.59
1:D:368:GLN:H	1:D:371:HIS:CD2	2.20	0.58
1:G:368:GLN:H	1:G:371:HIS:CD2	2.20	0.58
1:D:155:VAL:HB	1:D:268:LEU:HD22	1.85	0.58
1:C:157:ILE:HB	1:C:270:THR:HG22	1.86	0.57
1:D:189:ALA:HB2	1:D:234:GLU:HG3	1.86	0.57
1:D:285:ARG:HA	2:D:401:EDO:H22	1.85	0.57
1:B:157:ILE:HB	1:B:270:THR:HG22	1.85	0.57
1:B:188:CYS:HB3	1:B:196:LEU:HD11	1.87	0.57
1:C:141:LEU:HD23	1:C:299:TRP:HE3	1.69	0.56
1:B:155:VAL:HB	1:B:268:LEU:HD22	1.87	0.56
1:A:155:VAL:HB	1:A:268:LEU:HD22	1.86	0.56
1:C:368:GLN:H	1:C:371:HIS:CD2	2.23	0.56
1:E:368:GLN:H	1:E:371:HIS:HD2	1.53	0.56
1:E:223:GLN:HE22	1:E:263:LEU:HD12	1.71	0.56
1:F:155:VAL:HB	1:F:268:LEU:HD22	1.88	0.56
1:F:367:ILE:HD12	1:F:372:ILE:HD11	1.89	0.55
1:A:368:GLN:H	1:A:371:HIS:CD2	2.25	0.55
1:F:287:ASP:N	1:F:287:ASP:OD1	2.40	0.55
1:G:300:PRO:HG2	1:G:305:ARG:HD3	1.89	0.55
1:A:258:ARG:H	1:A:258:ARG:CD	2.19	0.54
1:B:165:LYS:C	1:B:167:VAL:H	2.10	0.54
1:D:374:LEU:HD22	1:D:374:LEU:H	1.72	0.54
1:D:170:ARG:O	1:D:174:ASN:ND2	2.41	0.54
1:C:155:VAL:HB	1:C:268:LEU:HD22	1.87	0.54
1:D:321:CYS:HB2	1:D:328:VAL:HG12	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:GLU:O	1:F:166:GLU:HG2	2.08	0.53
1:F:367:ILE:HA	1:F:371:HIS:HD2	1.72	0.53
1:B:165:LYS:C	1:B:167:VAL:N	2.61	0.52
1:A:287:ASP:OD1	1:A:288:LEU:N	2.41	0.52
1:E:310:GLU:HG3	1:E:336:ILE:HD12	1.91	0.52
1:G:189:ALA:HB2	1:G:234:GLU:HG3	1.91	0.52
1:A:290:TYR:O	1:G:353:ASN:ND2	2.42	0.51
1:B:368:GLN:H	1:B:371:HIS:CD2	2.28	0.51
1:D:131:MET:SD	1:D:131:MET:N	2.82	0.51
1:D:287:ASP:OD1	1:D:288:LEU:N	2.44	0.51
1:D:357:ARG:NH1	1:D:373:LEU:O	2.44	0.51
1:D:360:ILE:HG21	1:E:148:VAL:HG13	1.92	0.51
1:B:368:GLN:H	1:B:371:HIS:HD2	1.57	0.51
1:A:258:ARG:CD	1:A:258:ARG:N	2.73	0.50
1:B:166:GLU:HG3	1:B:228:LEU:HD22	1.92	0.50
1:E:300:PRO:HG2	1:E:305:ARG:HD3	1.93	0.49
1:D:157:ILE:HB	1:D:270:THR:HG22	1.94	0.49
1:D:164:GLY:O	1:D:167:VAL:HG22	2.13	0.49
1:B:360:ILE:HG21	1:C:148:VAL:HG13	1.94	0.49
1:G:155:VAL:HB	1:G:268:LEU:HD22	1.95	0.49
1:F:368:GLN:H	1:F:371:HIS:CD2	2.30	0.48
1:C:300:PRO:HG2	1:C:305:ARG:HD3	1.95	0.48
1:B:287:ASP:OD1	1:B:288:LEU:N	2.47	0.48
1:E:164:GLY:HA2	1:E:167:VAL:HG22	1.96	0.48
1:F:141:LEU:HD23	1:F:299:TRP:CE3	2.46	0.48
1:F:160:PRO:HD2	1:F:299:TRP:O	2.14	0.48
1:B:199:THR:O	1:B:218:LYS:HG2	2.14	0.47
1:D:141:LEU:HD23	1:D:299:TRP:CE3	2.48	0.47
1:A:148:VAL:HG13	1:G:360:ILE:HG21	1.97	0.47
1:B:308:ASP:O	1:B:312:LEU:HB2	2.14	0.47
1:A:362:SER:HB3	1:A:371:HIS:CD2	2.50	0.47
1:C:164:GLY:HA2	1:C:167:VAL:HG22	1.97	0.47
1:A:360:ILE:HG21	1:B:148:VAL:HG13	1.97	0.46
1:B:337:THR:O	1:B:341:ASN:ND2	2.39	0.46
1:C:130:HIS:CE1	1:C:174:ASN:HD22	2.33	0.46
1:F:331:ILE:HG13	1:F:367:ILE:HD11	1.97	0.46
1:F:130:HIS:HB3	1:F:131:MET:H	1.57	0.46
1:G:132:VAL:HG23	1:G:133:VAL:H	1.81	0.46
1:A:258:ARG:HD2	1:A:258:ARG:N	2.20	0.46
1:G:166:GLU:OE2	1:G:170:ARG:NH2	2.49	0.46
1:D:300:PRO:HG2	1:D:305:ARG:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ALA:O	1:B:317:ILE:HG13	2.16	0.45
1:A:223:GLN:NE2	1:A:262:LYS:O	2.50	0.45
1:A:318:GLU:O	1:A:322:LYS:HG2	2.17	0.45
1:E:308:ASP:O	1:E:312:LEU:HB2	2.17	0.45
1:A:316:LEU:O	1:A:320:HIS:HB2	2.17	0.44
1:A:368:GLN:H	1:A:371:HIS:HD2	1.66	0.44
1:A:300:PRO:HG2	1:A:305:ARG:HD3	1.99	0.44
1:D:328:VAL:HA	1:D:329:PRO:HD3	1.83	0.44
1:E:262:LYS:HD3	1:E:262:LYS:HA	1.85	0.44
1:F:164:GLY:O	1:F:167:VAL:N	2.47	0.44
1:C:360:ILE:HG21	1:D:148:VAL:HG13	1.99	0.44
1:G:133:VAL:HG21	1:G:142:LEU:HD12	1.99	0.44
1:C:141:LEU:HD23	1:C:299:TRP:CE3	2.51	0.44
1:D:252:VAL:HB	1:D:263:LEU:HD11	2.00	0.44
1:G:142:LEU:HD23	1:G:142:LEU:HA	1.87	0.43
1:G:131:MET:HE1	1:G:168:MET:HA	2.00	0.43
1:E:287:ASP:OD1	1:E:288:LEU:N	2.52	0.43
1:C:367:ILE:HA	1:C:371:HIS:HD2	1.84	0.43
1:E:310:GLU:HB3	1:E:311:PRO:HD3	1.99	0.43
1:G:287:ASP:OD1	1:G:288:LEU:N	2.52	0.43
1:B:236:ASP:OD1	1:B:239:LEU:HB2	2.19	0.43
1:F:157:ILE:HG22	1:F:165:LYS:HD3	2.01	0.43
1:F:189:ALA:HB2	1:F:234:GLU:HG3	2.00	0.43
1:A:252:VAL:HB	1:A:263:LEU:HD11	2.01	0.43
1:G:310:GLU:HB3	1:G:311:PRO:HD3	2.01	0.43
1:G:187:ASN:HA	1:G:230:ASP:HB3	2.00	0.42
1:C:148:VAL:O	1:C:266:ARG:NH2	2.53	0.42
1:D:310:GLU:HB3	1:D:311:PRO:HD3	2.01	0.42
1:E:203:TYR:OH	1:F:258:ARG:NH1	2.52	0.42
1:B:130:HIS:HB3	1:B:131:MET:H	1.52	0.42
1:F:342:TYR:CD1	1:F:343:PRO:HD2	2.54	0.42
1:A:286:GLU:H	2:A:401:EDO:H11	1.83	0.42
1:C:316:LEU:HD13	1:C:352:ASP:HA	2.01	0.42
1:F:303:CYS:HB3	1:F:343:PRO:O	2.20	0.42
1:G:169:SER:H	1:G:169:SER:HG	1.52	0.42
1:A:342:TYR:CD1	1:A:343:PRO:HD2	2.55	0.42
1:A:357:ARG:NH1	1:A:373:LEU:O	2.53	0.42
1:C:223:GLN:HE22	1:C:263:LEU:HD23	1.85	0.42
1:E:165:LYS:HE3	1:E:270:THR:HG23	2.02	0.42
1:G:313:ALA:O	1:G:317:ILE:HG13	2.20	0.42
1:F:318:GLU:HG2	1:F:328:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:251:GLU:HG3	1:G:260:SER:HB3	2.01	0.42
1:B:285:ARG:HA	2:B:401:EDO:H12	2.02	0.41
1:B:187:ASN:HA	1:B:230:ASP:HB3	2.02	0.41
1:B:328:VAL:HA	1:B:329:PRO:HD3	1.80	0.41
1:E:342:TYR:CD1	1:E:343:PRO:HD2	2.55	0.41
1:D:161:SER:OG	1:D:231:GLU:OE2	2.32	0.41
1:G:165:LYS:O	1:G:169:SER:OG	2.32	0.41
1:F:300:PRO:HG2	1:F:305:ARG:HD3	2.02	0.41
1:F:316:LEU:HD13	1:F:352:ASP:HA	2.01	0.41
1:A:316:LEU:HD13	1:A:352:ASP:HA	2.02	0.41
1:F:191:ILE:HA	1:F:192:PRO:HD3	1.81	0.41
1:D:238:ASN:O	1:D:242:LYS:HG3	2.21	0.41
1:F:367:ILE:O	1:F:367:ILE:HG13	2.21	0.41
1:B:244:LEU:O	1:B:248:GLN:HG3	2.21	0.40
1:C:362:SER:HB3	1:C:371:HIS:CD2	2.55	0.40
1:A:159:GLY:O	1:A:272:ASN:HA	2.21	0.40
1:A:303:CYS:HB3	1:A:343:PRO:O	2.21	0.40
1:G:164:GLY:O	1:G:167:VAL:HG12	2.21	0.40
1:C:191:ILE:HA	1:C:192:PRO:HD3	1.84	0.40
1:D:372:ILE:HG22	1:D:374:LEU:HD13	2.04	0.40
1:D:178:ARG:NH2	1:D:264:ASP:O	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ALA:O	1:E:205:LYS:NZ[4_455]	2.00	0.20

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	245/271 (90%)	233 (95%)	12 (5%)	0	100	100
1	B	245/271 (90%)	232 (95%)	11 (4%)	2 (1%)	19	54
1	C	246/271 (91%)	230 (94%)	13 (5%)	3 (1%)	13	44
1	D	244/271 (90%)	231 (95%)	12 (5%)	1 (0%)	34	69
1	E	244/271 (90%)	234 (96%)	10 (4%)	0	100	100
1	F	245/271 (90%)	231 (94%)	14 (6%)	0	100	100
1	G	244/271 (90%)	231 (95%)	11 (4%)	2 (1%)	19	54
All	All	1713/1897 (90%)	1622 (95%)	83 (5%)	8 (0%)	29	64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	166	GLU
1	G	133	VAL
1	D	132	VAL
1	B	165	LYS
1	C	131	MET
1	G	209	THR
1	C	370	GLU
1	C	132	VAL

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	208/229 (91%)	194 (93%)	14 (7%)	16	46
1	B	208/229 (91%)	189 (91%)	19 (9%)	9	33
1	C	209/229 (91%)	203 (97%)	6 (3%)	42	72
1	D	207/229 (90%)	191 (92%)	16 (8%)	13	41
1	E	207/229 (90%)	188 (91%)	19 (9%)	9	33
1	F	208/229 (91%)	194 (93%)	14 (7%)	16	46
1	G	207/229 (90%)	188 (91%)	19 (9%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1454/1603 (91%)	1347 (93%)	107 (7%)	13 42

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	LEU
1	A	148	VAL
1	A	152	ASP
1	A	163	SER
1	A	170	ARG
1	A	239	LEU
1	A	250	ARG
1	A	258	ARG
1	A	260	SER
1	A	276	LYS
1	A	319	ARG
1	A	320	HIS
1	A	339	LEU
1	A	374	LEU
1	B	130	HIS
1	B	148	VAL
1	B	158	LEU
1	B	163	SER
1	B	168	MET
1	B	170	ARG
1	B	196	LEU
1	B	239	LEU
1	B	253	GLU
1	B	259	LYS
1	B	260	SER
1	B	266	ARG
1	B	293	ASN
1	B	298	THR
1	B	319	ARG
1	B	322	LYS
1	B	328	VAL
1	B	340	LEU
1	B	375	GLU
1	C	148	VAL
1	C	179	LYS
1	C	180	GLU
1	C	239	LEU

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Mol	Chain	Res	Type
1	C	266	ARG
1	C	368	GLN
1	D	131	MET
1	D	148	VAL
1	D	161	SER
1	D	163	SER
1	D	230	ASP
1	D	239	LEU
1	D	253	GLU
1	D	258	ARG
1	D	260	SER
1	D	266	ARG
1	D	322	LYS
1	D	326	LEU
1	D	353	ASN
1	D	361	LEU
1	D	370	GLU
1	D	374	LEU
1	E	132	VAL
1	E	141	LEU
1	E	144	LEU
1	E	148	VAL
1	E	163	SER
1	E	169	SER
1	E	170	ARG
1	E	230	ASP
1	E	245	ARG
1	E	258	ARG
1	E	263	LEU
1	E	266	ARG
1	E	270	THR
1	E	312	LEU
1	E	319	ARG
1	E	324	LEU
1	E	326	LEU
1	E	355	VAL
1	E	364	ASN
1	F	161	SER
1	F	163	SER
1	F	179	LYS
1	F	249	GLU
1	F	258	ARG

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Mol	Chain	Res	Type
1	F	266	ARG
1	F	277	GLN
1	F	294	VAL
1	F	319	ARG
1	F	320	HIS
1	F	361	LEU
1	F	367	ILE
1	F	370	GLU
1	F	374	LEU
1	G	132	VAL
1	G	156	MET
1	G	167	VAL
1	G	169	SER
1	G	179	LYS
1	G	180	GLU
1	G	209	THR
1	G	230	ASP
1	G	231	GLU
1	G	239	LEU
1	G	251	GLU
1	G	266	ARG
1	G	270	THR
1	G	277	GLN
1	G	319	ARG
1	G	324	LEU
1	G	326	LEU
1	G	363	GLU
1	G	364	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
1	A	371	HIS
1	B	368	GLN
1	B	371	HIS
1	C	130	HIS
1	C	371	HIS
1	D	174	ASN
1	D	371	HIS
1	E	368	GLN
1	E	371	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	130	HIS
1	F	174	ASN
1	F	371	HIS
1	G	368	GLN
1	G	371	HIS

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

7 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	EDO	G	401	-	3,3,3	0.46	0	2,2,2	0.36	0
2	EDO	B	401	-	3,3,3	0.47	0	2,2,2	0.31	0
2	EDO	D	401	-	3,3,3	0.47	0	2,2,2	0.37	0
2	EDO	E	401	-	3,3,3	0.47	0	2,2,2	0.31	0
2	EDO	A	401	-	3,3,3	0.49	0	2,2,2	0.26	0
2	EDO	F	401	-	3,3,3	0.50	0	2,2,2	0.22	0
2	EDO	C	401	-	3,3,3	0.51	0	2,2,2	0.19	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
2	EDO	G	401	-	-	0/1/1/1	-
2	EDO	B	401	-	-	0/1/1/1	-
2	EDO	D	401	-	-	0/1/1/1	-
2	EDO	E	401	-	-	0/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	F	401	-	-	0/1/1/1	-
2	EDO	C	401	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

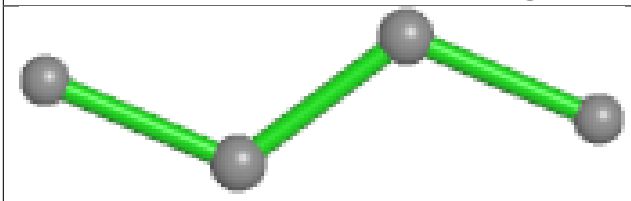
There are no ring outliers.

4 monomers are involved in 4 short contacts:

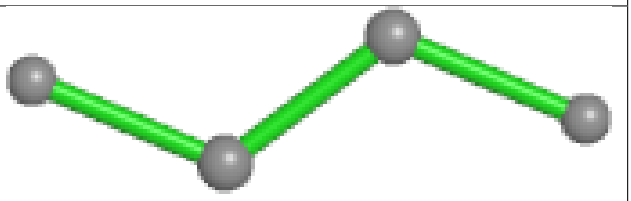
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	EDO	1	0
2	D	401	EDO	1	0
2	E	401	EDO	1	0
2	A	401	EDO	1	0

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.

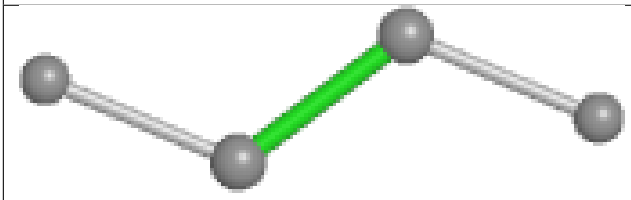
Ligand EDO G 401



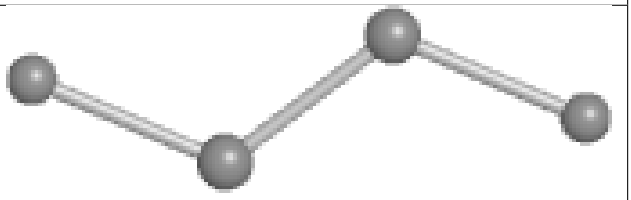
Bond lengths



Bond angles

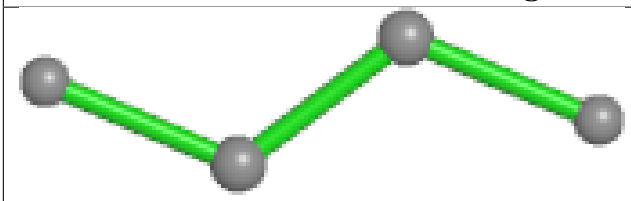


Torsions

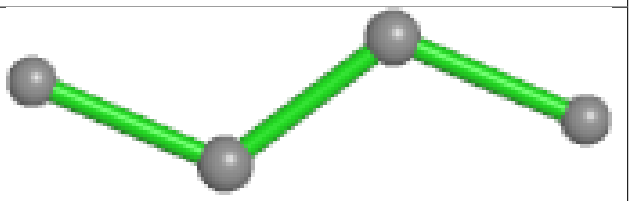


Rings

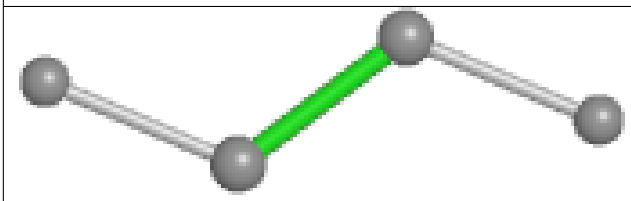
Ligand EDO B 401



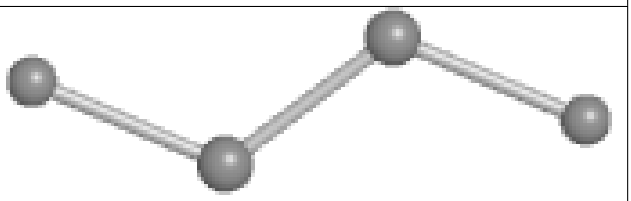
Bond lengths



Bond angles

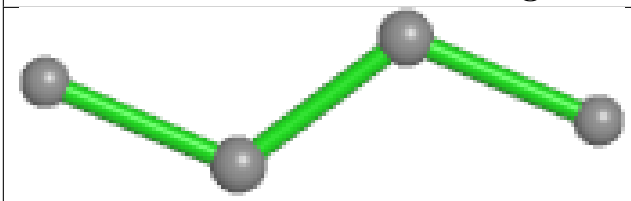


Torsions

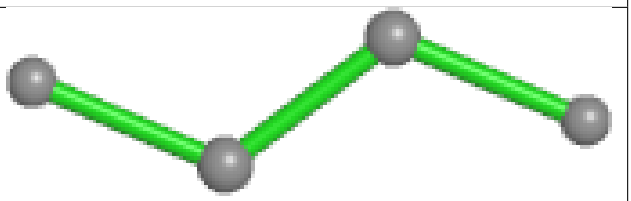


Rings

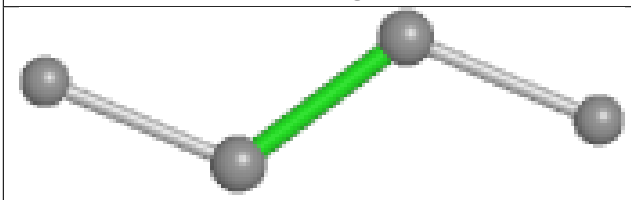
Ligand EDO D 401



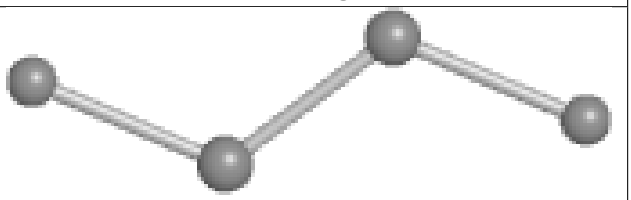
Bond lengths



Bond angles

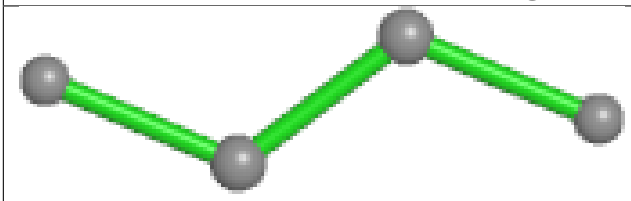


Torsions

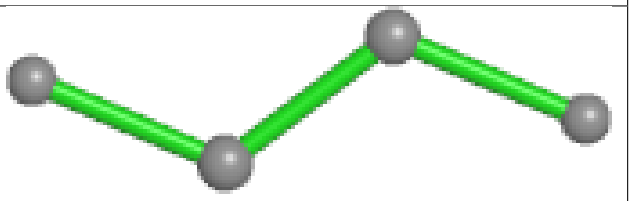


Rings

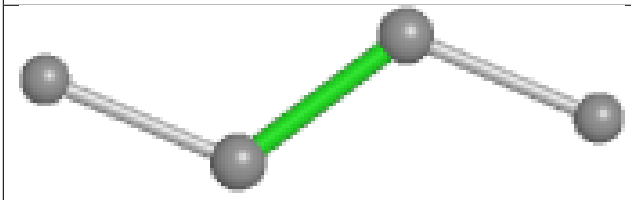
Ligand EDO E 401



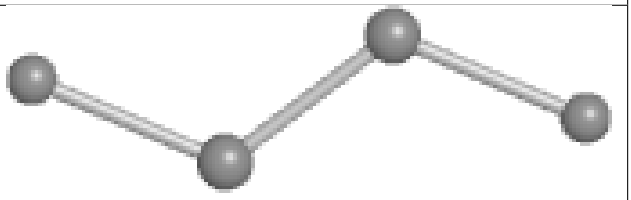
Bond lengths



Bond angles

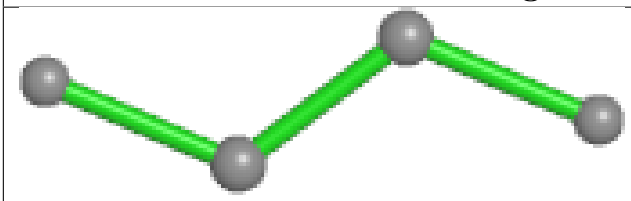


Torsions

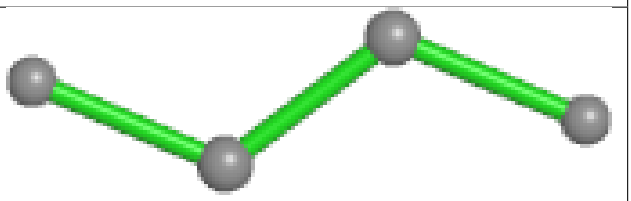


Rings

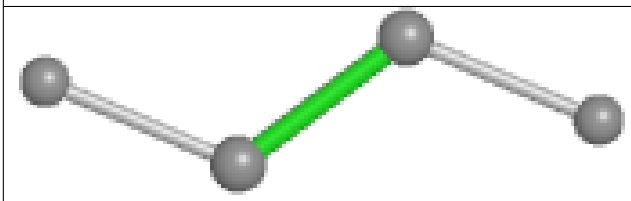
Ligand EDO A 401



Bond lengths



Bond angles



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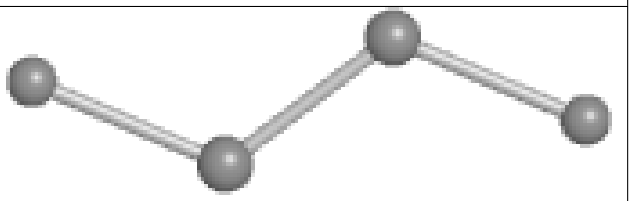
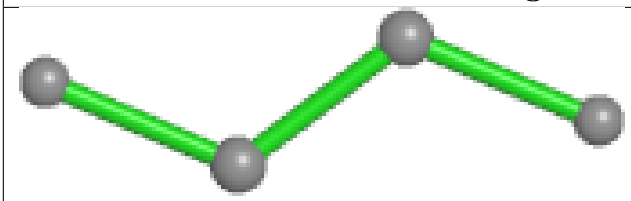
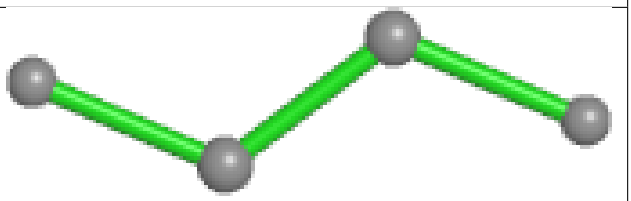


Rings

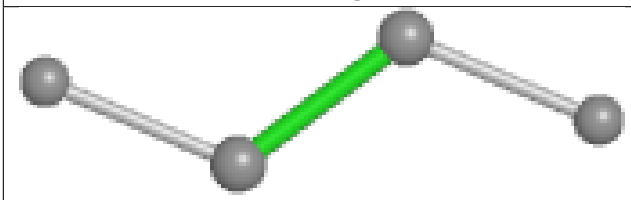
Ligand EDO F 401



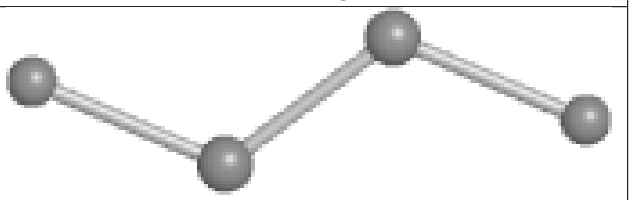
Bond lengths



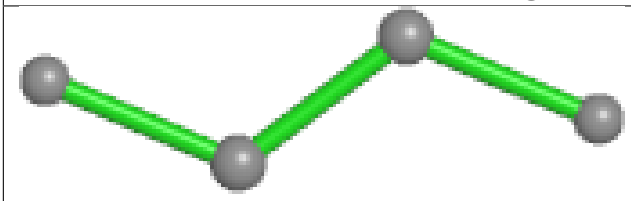
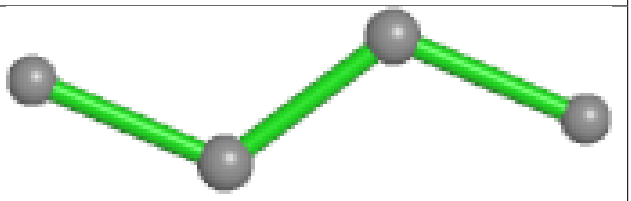
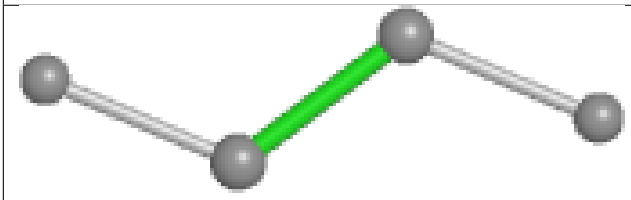
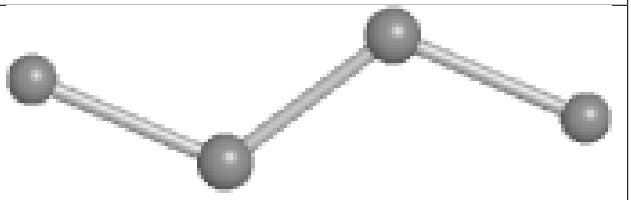
Bond angles



Torsions



Rings

Ligand EDO C 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	247/271 (91%)	-0.51	0 100 100	23, 40, 74, 109	0
1	B	247/271 (91%)	-0.55	1 (0%) 92 84	25, 37, 58, 98	0
1	C	247/271 (91%)	-0.48	0 100 100	21, 40, 68, 85	0
1	D	246/271 (90%)	-0.49	0 100 100	24, 37, 58, 95	0
1	E	246/271 (90%)	-0.53	0 100 100	20, 34, 57, 81	0
1	F	247/271 (91%)	-0.48	0 100 100	21, 41, 71, 97	0
1	G	246/271 (90%)	-0.56	0 100 100	20, 36, 55, 84	0
All	All	1726/1897 (90%)	-0.52	1 (0%) 95 92	20, 38, 64, 109	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	131	MET	2.2

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 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,

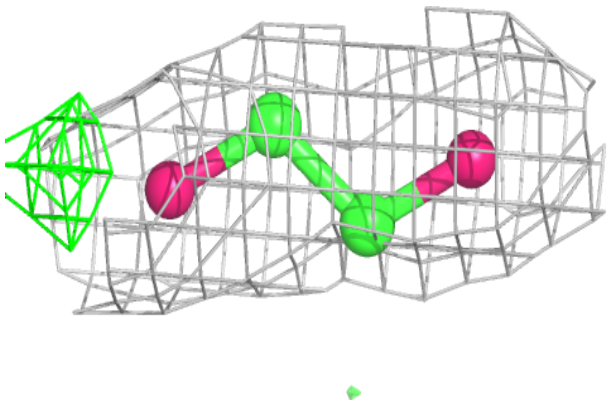
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

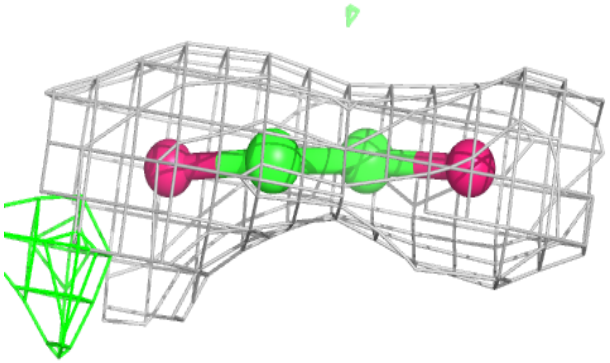
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	F	401	4/4	0.77	0.29	31,46,54,56	0
2	EDO	C	401	4/4	0.81	0.36	40,53,59,64	0
2	EDO	E	401	4/4	0.83	0.30	38,50,53,54	0
2	EDO	D	401	4/4	0.83	0.25	42,45,46,47	0
2	EDO	A	401	4/4	0.86	0.30	30,46,51,54	0
2	EDO	B	401	4/4	0.86	0.24	30,42,42,45	0
2	EDO	G	401	4/4	0.90	0.27	48,48,48,57	0

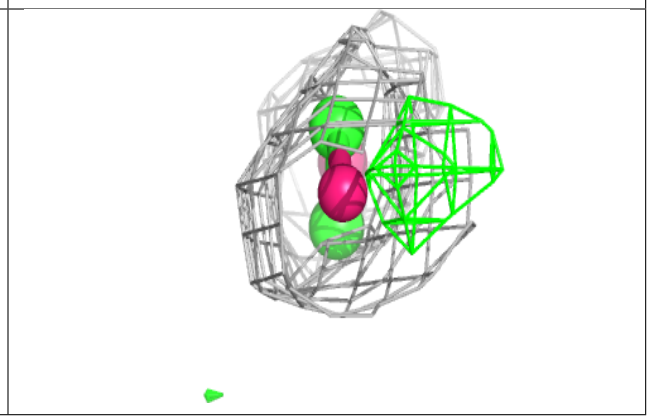
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EDO F 401:

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

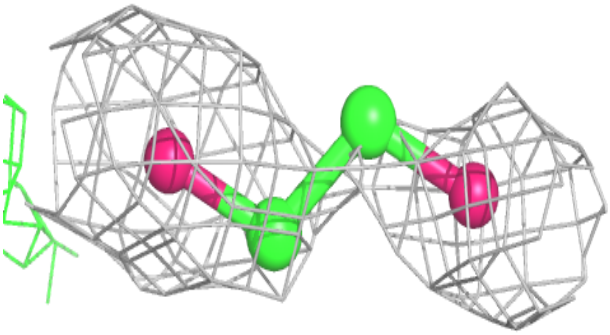


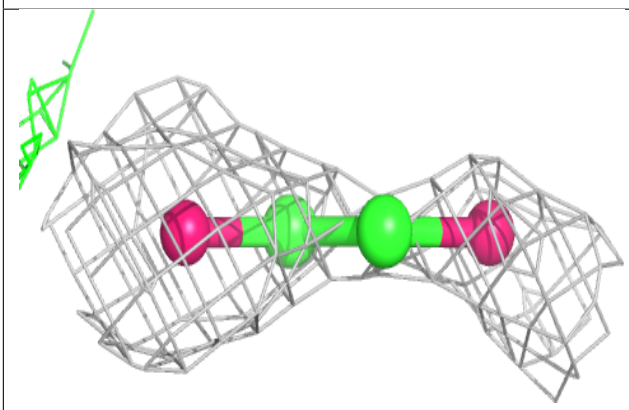


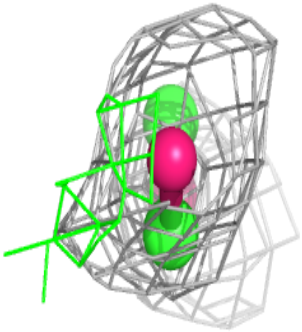


Electron density around EDO C 401:

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

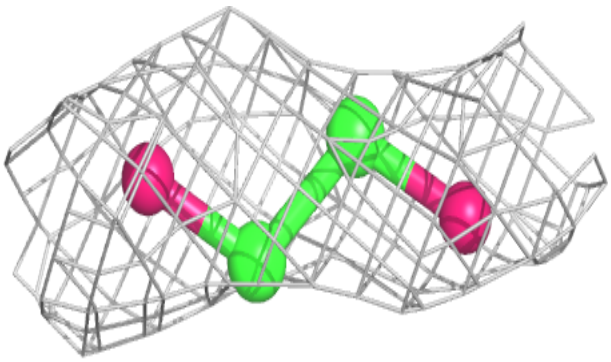


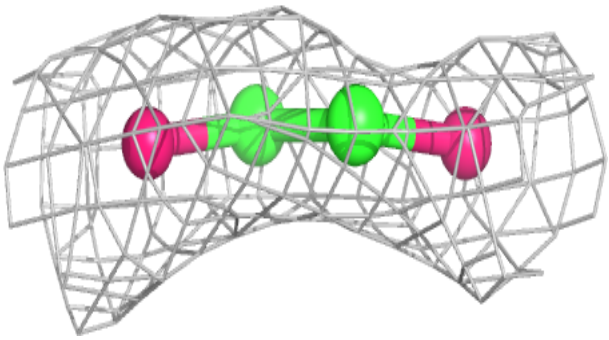


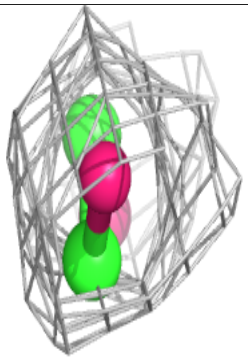


Electron density around EDO E 401:

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

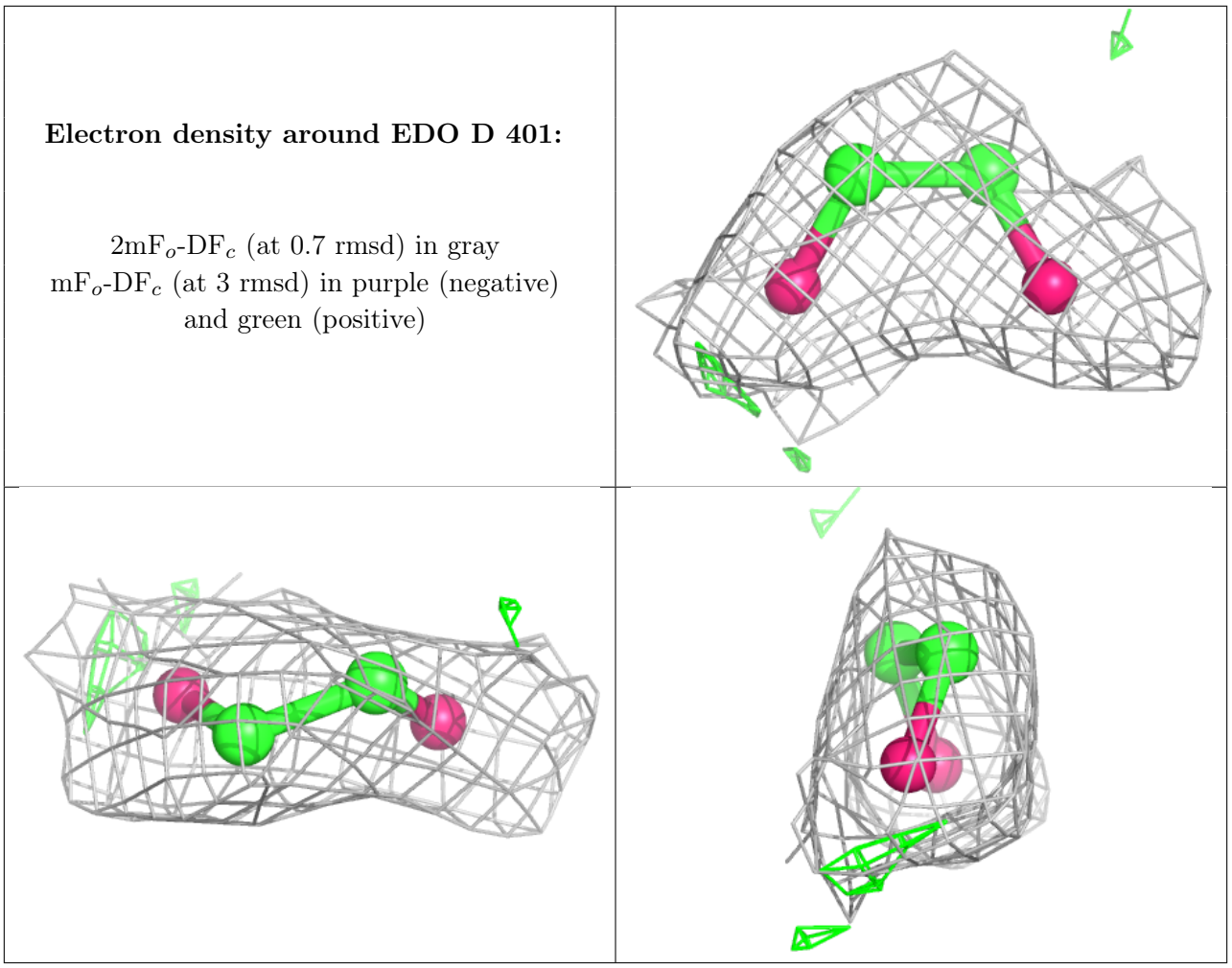






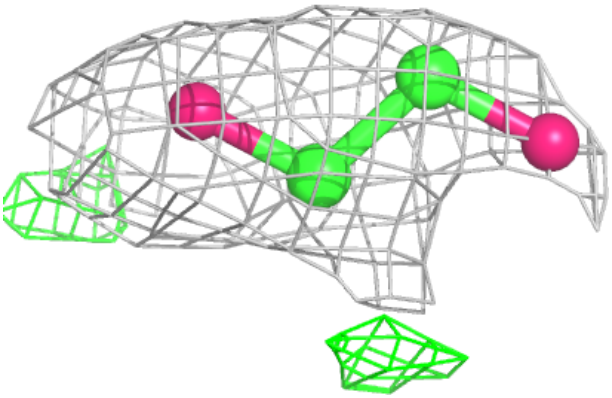
Electron density around EDO D 401:

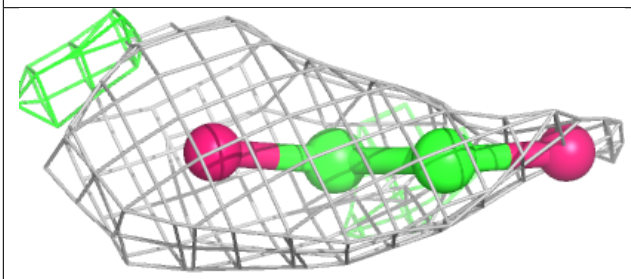
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

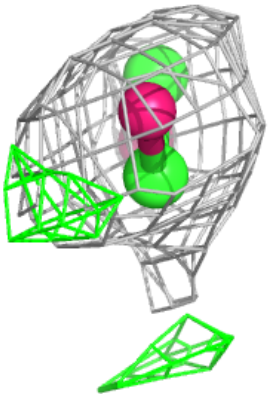


Electron density around EDO A 401:

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

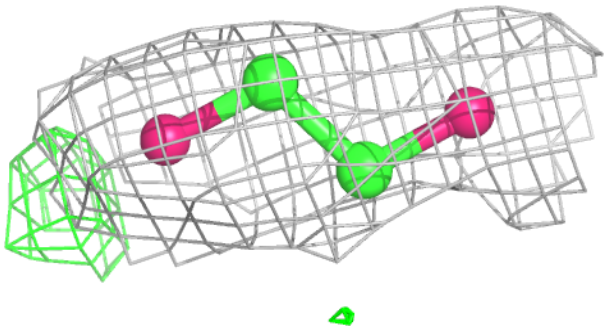


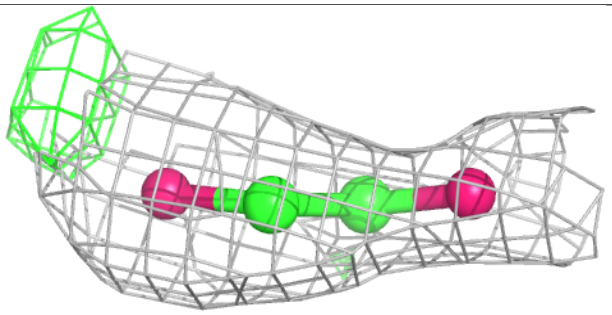


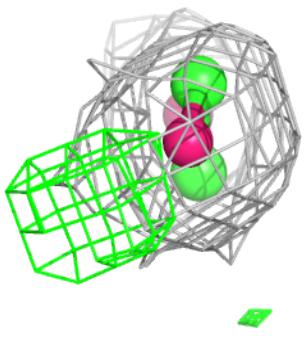


Electron density around EDO B 401:

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

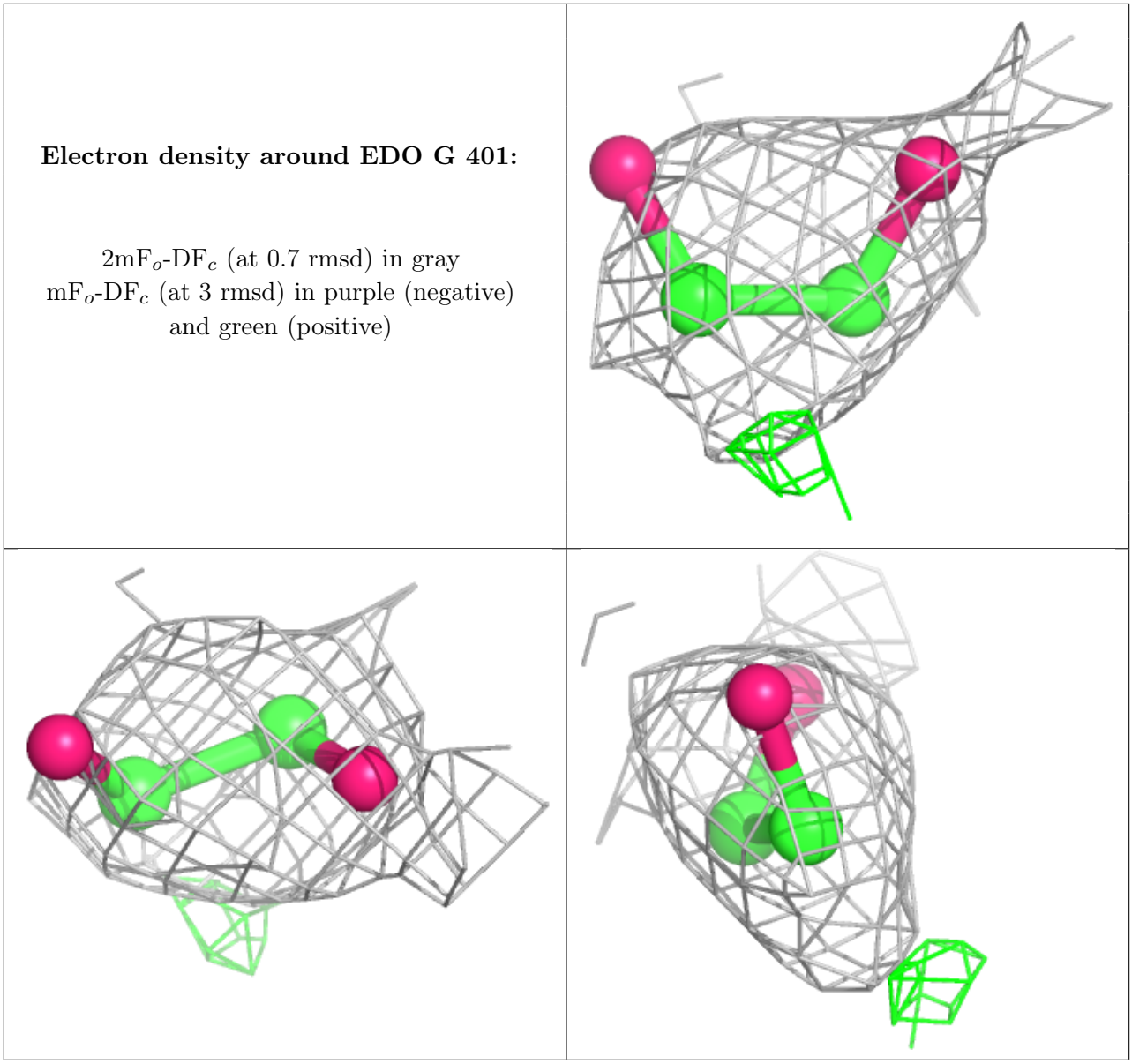






Electron density around EDO G 401:

$2mF_o$-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

There are no such residues in this entry.