Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 07:01 PM JST

PDB ID	:	7XRV
Title	:	Bacteroides thetaiotaomicron ferulic acid esterase - S150A (BT_4077-S150A) complex with trans-methylferulate
Authors	:	Du, G.M.; Wang, Y.L.; Xin, F.J.
Deposited on	:	2022-05-11
Resolution	:	2.71 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:

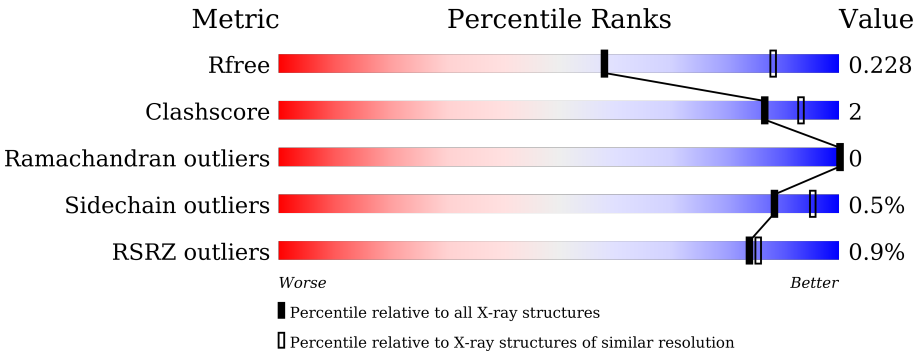
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	291	84% 8% 8%
1	B	291	86% 6% 8%
1	C	291	86% 5% 8%
1	D	291	89% 8%
1	E	291	90% 8%
1	F	291	87% 5% 8%

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Mol	Chain	Length	Quality of chain
1	G	291	88% 8%
1	H	291	2% 86% 6% 8%
1	I	291	% 88% 8%
1	J	291	% 86% 6% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SZQ	A	302	-	X	-	-
3	SZQ	F	302	-	X	-	-
3	SZQ	G	302	-	X	-	-
3	SZQ	H	302	-	X	-	-
3	SZQ	I	302	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22132 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 Ferulic acid esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2160	1389	362	397	12			
1	B	268	Total	C	N	O	S	4	1	0
			2164	1392	362	398	12			
1	C	268	Total	C	N	O	S	0	0	0
			2160	1390	361	397	12			
1	D	268	Total	C	N	O	S	0	0	0
			2151	1385	360	394	12			
1	E	268	Total	C	N	O	S	0	0	0
			2160	1389	361	398	12			
1	F	268	Total	C	N	O	S	0	0	0
			2152	1385	360	395	12			
1	G	268	Total	C	N	O	S	0	0	0
			2152	1385	360	395	12			
1	H	268	Total	C	N	O	S	0	0	0
			2152	1385	360	395	12			
1	I	268	Total	C	N	O	S	0	0	0
			2152	1385	360	395	12			
1	J	268	Total	C	N	O	S	0	0	0
			2152	1385	360	395	12			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP Q8A0E4
A	-1	GLY	-	expression tag	UNP Q8A0E4
A	0	SER	-	expression tag	UNP Q8A0E4
A	1	SER	-	expression tag	UNP Q8A0E4
A	2	HIS	-	expression tag	UNP Q8A0E4
A	3	HIS	-	expression tag	UNP Q8A0E4
A	4	HIS	-	expression tag	UNP Q8A0E4
A	5	HIS	-	expression tag	UNP Q8A0E4
A	6	HIS	-	expression tag	UNP Q8A0E4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	7	HIS	-	expression tag	UNP Q8A0E4
A	8	SER	-	expression tag	UNP Q8A0E4
A	9	SER	-	expression tag	UNP Q8A0E4
A	10	GLY	-	expression tag	UNP Q8A0E4
A	11	LEU	-	expression tag	UNP Q8A0E4
A	12	VAL	-	expression tag	UNP Q8A0E4
A	13	PRO	-	expression tag	UNP Q8A0E4
A	14	ARG	-	expression tag	UNP Q8A0E4
A	15	GLY	-	expression tag	UNP Q8A0E4
A	16	SER	-	expression tag	UNP Q8A0E4
A	17	HIS	-	expression tag	UNP Q8A0E4
A	18	MET	-	expression tag	UNP Q8A0E4
A	19	LEU	-	expression tag	UNP Q8A0E4
A	20	GLU	-	expression tag	UNP Q8A0E4
A	150	ALA	SER	engineered mutation	UNP Q8A0E4
B	-2	MET	-	initiating methionine	UNP Q8A0E4
B	-1	GLY	-	expression tag	UNP Q8A0E4
B	0	SER	-	expression tag	UNP Q8A0E4
B	1	SER	-	expression tag	UNP Q8A0E4
B	2	HIS	-	expression tag	UNP Q8A0E4
B	3	HIS	-	expression tag	UNP Q8A0E4
B	4	HIS	-	expression tag	UNP Q8A0E4
B	5	HIS	-	expression tag	UNP Q8A0E4
B	6	HIS	-	expression tag	UNP Q8A0E4
B	7	HIS	-	expression tag	UNP Q8A0E4
B	8	SER	-	expression tag	UNP Q8A0E4
B	9	SER	-	expression tag	UNP Q8A0E4
B	10	GLY	-	expression tag	UNP Q8A0E4
B	11	LEU	-	expression tag	UNP Q8A0E4
B	12	VAL	-	expression tag	UNP Q8A0E4
B	13	PRO	-	expression tag	UNP Q8A0E4
B	14	ARG	-	expression tag	UNP Q8A0E4
B	15	GLY	-	expression tag	UNP Q8A0E4
B	16	SER	-	expression tag	UNP Q8A0E4
B	17	HIS	-	expression tag	UNP Q8A0E4
B	18	MET	-	expression tag	UNP Q8A0E4
B	19	LEU	-	expression tag	UNP Q8A0E4
B	20	GLU	-	expression tag	UNP Q8A0E4
B	150	ALA	SER	engineered mutation	UNP Q8A0E4
C	-2	MET	-	initiating methionine	UNP Q8A0E4
C	-1	GLY	-	expression tag	UNP Q8A0E4
C	0	SER	-	expression tag	UNP Q8A0E4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	SER	-	expression tag	UNP Q8A0E4
C	2	HIS	-	expression tag	UNP Q8A0E4
C	3	HIS	-	expression tag	UNP Q8A0E4
C	4	HIS	-	expression tag	UNP Q8A0E4
C	5	HIS	-	expression tag	UNP Q8A0E4
C	6	HIS	-	expression tag	UNP Q8A0E4
C	7	HIS	-	expression tag	UNP Q8A0E4
C	8	SER	-	expression tag	UNP Q8A0E4
C	9	SER	-	expression tag	UNP Q8A0E4
C	10	GLY	-	expression tag	UNP Q8A0E4
C	11	LEU	-	expression tag	UNP Q8A0E4
C	12	VAL	-	expression tag	UNP Q8A0E4
C	13	PRO	-	expression tag	UNP Q8A0E4
C	14	ARG	-	expression tag	UNP Q8A0E4
C	15	GLY	-	expression tag	UNP Q8A0E4
C	16	SER	-	expression tag	UNP Q8A0E4
C	17	HIS	-	expression tag	UNP Q8A0E4
C	18	MET	-	expression tag	UNP Q8A0E4
C	19	LEU	-	expression tag	UNP Q8A0E4
C	20	GLU	-	expression tag	UNP Q8A0E4
C	150	ALA	SER	engineered mutation	UNP Q8A0E4
D	-2	MET	-	initiating methionine	UNP Q8A0E4
D	-1	GLY	-	expression tag	UNP Q8A0E4
D	0	SER	-	expression tag	UNP Q8A0E4
D	1	SER	-	expression tag	UNP Q8A0E4
D	2	HIS	-	expression tag	UNP Q8A0E4
D	3	HIS	-	expression tag	UNP Q8A0E4
D	4	HIS	-	expression tag	UNP Q8A0E4
D	5	HIS	-	expression tag	UNP Q8A0E4
D	6	HIS	-	expression tag	UNP Q8A0E4
D	7	HIS	-	expression tag	UNP Q8A0E4
D	8	SER	-	expression tag	UNP Q8A0E4
D	9	SER	-	expression tag	UNP Q8A0E4
D	10	GLY	-	expression tag	UNP Q8A0E4
D	11	LEU	-	expression tag	UNP Q8A0E4
D	12	VAL	-	expression tag	UNP Q8A0E4
D	13	PRO	-	expression tag	UNP Q8A0E4
D	14	ARG	-	expression tag	UNP Q8A0E4
D	15	GLY	-	expression tag	UNP Q8A0E4
D	16	SER	-	expression tag	UNP Q8A0E4
D	17	HIS	-	expression tag	UNP Q8A0E4
D	18	MET	-	expression tag	UNP Q8A0E4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	19	LEU	-	expression tag	UNP Q8A0E4
D	20	GLU	-	expression tag	UNP Q8A0E4
D	150	ALA	SER	engineered mutation	UNP Q8A0E4
E	-2	MET	-	initiating methionine	UNP Q8A0E4
E	-1	GLY	-	expression tag	UNP Q8A0E4
E	0	SER	-	expression tag	UNP Q8A0E4
E	1	SER	-	expression tag	UNP Q8A0E4
E	2	HIS	-	expression tag	UNP Q8A0E4
E	3	HIS	-	expression tag	UNP Q8A0E4
E	4	HIS	-	expression tag	UNP Q8A0E4
E	5	HIS	-	expression tag	UNP Q8A0E4
E	6	HIS	-	expression tag	UNP Q8A0E4
E	7	HIS	-	expression tag	UNP Q8A0E4
E	8	SER	-	expression tag	UNP Q8A0E4
E	9	SER	-	expression tag	UNP Q8A0E4
E	10	GLY	-	expression tag	UNP Q8A0E4
E	11	LEU	-	expression tag	UNP Q8A0E4
E	12	VAL	-	expression tag	UNP Q8A0E4
E	13	PRO	-	expression tag	UNP Q8A0E4
E	14	ARG	-	expression tag	UNP Q8A0E4
E	15	GLY	-	expression tag	UNP Q8A0E4
E	16	SER	-	expression tag	UNP Q8A0E4
E	17	HIS	-	expression tag	UNP Q8A0E4
E	18	MET	-	expression tag	UNP Q8A0E4
E	19	LEU	-	expression tag	UNP Q8A0E4
E	20	GLU	-	expression tag	UNP Q8A0E4
E	150	ALA	SER	engineered mutation	UNP Q8A0E4
F	-2	MET	-	initiating methionine	UNP Q8A0E4
F	-1	GLY	-	expression tag	UNP Q8A0E4
F	0	SER	-	expression tag	UNP Q8A0E4
F	1	SER	-	expression tag	UNP Q8A0E4
F	2	HIS	-	expression tag	UNP Q8A0E4
F	3	HIS	-	expression tag	UNP Q8A0E4
F	4	HIS	-	expression tag	UNP Q8A0E4
F	5	HIS	-	expression tag	UNP Q8A0E4
F	6	HIS	-	expression tag	UNP Q8A0E4
F	7	HIS	-	expression tag	UNP Q8A0E4
F	8	SER	-	expression tag	UNP Q8A0E4
F	9	SER	-	expression tag	UNP Q8A0E4
F	10	GLY	-	expression tag	UNP Q8A0E4
F	11	LEU	-	expression tag	UNP Q8A0E4
F	12	VAL	-	expression tag	UNP Q8A0E4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	13	PRO	-	expression tag	UNP Q8A0E4
F	14	ARG	-	expression tag	UNP Q8A0E4
F	15	GLY	-	expression tag	UNP Q8A0E4
F	16	SER	-	expression tag	UNP Q8A0E4
F	17	HIS	-	expression tag	UNP Q8A0E4
F	18	MET	-	expression tag	UNP Q8A0E4
F	19	LEU	-	expression tag	UNP Q8A0E4
F	20	GLU	-	expression tag	UNP Q8A0E4
F	150	ALA	SER	engineered mutation	UNP Q8A0E4
G	-2	MET	-	initiating methionine	UNP Q8A0E4
G	-1	GLY	-	expression tag	UNP Q8A0E4
G	0	SER	-	expression tag	UNP Q8A0E4
G	1	SER	-	expression tag	UNP Q8A0E4
G	2	HIS	-	expression tag	UNP Q8A0E4
G	3	HIS	-	expression tag	UNP Q8A0E4
G	4	HIS	-	expression tag	UNP Q8A0E4
G	5	HIS	-	expression tag	UNP Q8A0E4
G	6	HIS	-	expression tag	UNP Q8A0E4
G	7	HIS	-	expression tag	UNP Q8A0E4
G	8	SER	-	expression tag	UNP Q8A0E4
G	9	SER	-	expression tag	UNP Q8A0E4
G	10	GLY	-	expression tag	UNP Q8A0E4
G	11	LEU	-	expression tag	UNP Q8A0E4
G	12	VAL	-	expression tag	UNP Q8A0E4
G	13	PRO	-	expression tag	UNP Q8A0E4
G	14	ARG	-	expression tag	UNP Q8A0E4
G	15	GLY	-	expression tag	UNP Q8A0E4
G	16	SER	-	expression tag	UNP Q8A0E4
G	17	HIS	-	expression tag	UNP Q8A0E4
G	18	MET	-	expression tag	UNP Q8A0E4
G	19	LEU	-	expression tag	UNP Q8A0E4
G	20	GLU	-	expression tag	UNP Q8A0E4
G	150	ALA	SER	engineered mutation	UNP Q8A0E4
H	-2	MET	-	initiating methionine	UNP Q8A0E4
H	-1	GLY	-	expression tag	UNP Q8A0E4
H	0	SER	-	expression tag	UNP Q8A0E4
H	1	SER	-	expression tag	UNP Q8A0E4
H	2	HIS	-	expression tag	UNP Q8A0E4
H	3	HIS	-	expression tag	UNP Q8A0E4
H	4	HIS	-	expression tag	UNP Q8A0E4
H	5	HIS	-	expression tag	UNP Q8A0E4
H	6	HIS	-	expression tag	UNP Q8A0E4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	7	HIS	-	expression tag	UNP Q8A0E4
H	8	SER	-	expression tag	UNP Q8A0E4
H	9	SER	-	expression tag	UNP Q8A0E4
H	10	GLY	-	expression tag	UNP Q8A0E4
H	11	LEU	-	expression tag	UNP Q8A0E4
H	12	VAL	-	expression tag	UNP Q8A0E4
H	13	PRO	-	expression tag	UNP Q8A0E4
H	14	ARG	-	expression tag	UNP Q8A0E4
H	15	GLY	-	expression tag	UNP Q8A0E4
H	16	SER	-	expression tag	UNP Q8A0E4
H	17	HIS	-	expression tag	UNP Q8A0E4
H	18	MET	-	expression tag	UNP Q8A0E4
H	19	LEU	-	expression tag	UNP Q8A0E4
H	20	GLU	-	expression tag	UNP Q8A0E4
H	150	ALA	SER	engineered mutation	UNP Q8A0E4
I	-2	MET	-	initiating methionine	UNP Q8A0E4
I	-1	GLY	-	expression tag	UNP Q8A0E4
I	0	SER	-	expression tag	UNP Q8A0E4
I	1	SER	-	expression tag	UNP Q8A0E4
I	2	HIS	-	expression tag	UNP Q8A0E4
I	3	HIS	-	expression tag	UNP Q8A0E4
I	4	HIS	-	expression tag	UNP Q8A0E4
I	5	HIS	-	expression tag	UNP Q8A0E4
I	6	HIS	-	expression tag	UNP Q8A0E4
I	7	HIS	-	expression tag	UNP Q8A0E4
I	8	SER	-	expression tag	UNP Q8A0E4
I	9	SER	-	expression tag	UNP Q8A0E4
I	10	GLY	-	expression tag	UNP Q8A0E4
I	11	LEU	-	expression tag	UNP Q8A0E4
I	12	VAL	-	expression tag	UNP Q8A0E4
I	13	PRO	-	expression tag	UNP Q8A0E4
I	14	ARG	-	expression tag	UNP Q8A0E4
I	15	GLY	-	expression tag	UNP Q8A0E4
I	16	SER	-	expression tag	UNP Q8A0E4
I	17	HIS	-	expression tag	UNP Q8A0E4
I	18	MET	-	expression tag	UNP Q8A0E4
I	19	LEU	-	expression tag	UNP Q8A0E4
I	20	GLU	-	expression tag	UNP Q8A0E4
I	150	ALA	SER	engineered mutation	UNP Q8A0E4
J	-2	MET	-	initiating methionine	UNP Q8A0E4
J	-1	GLY	-	expression tag	UNP Q8A0E4
J	0	SER	-	expression tag	UNP Q8A0E4

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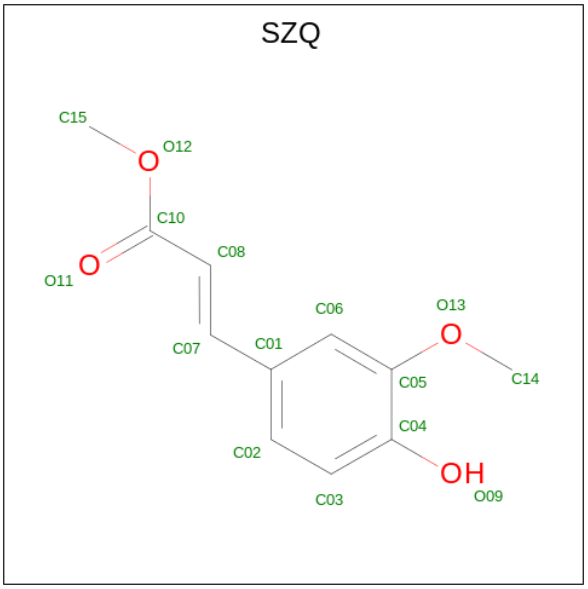
Chain	Residue	Modelled	Actual	Comment	Reference
J	1	SER	-	expression tag	UNP Q8A0E4
J	2	HIS	-	expression tag	UNP Q8A0E4
J	3	HIS	-	expression tag	UNP Q8A0E4
J	4	HIS	-	expression tag	UNP Q8A0E4
J	5	HIS	-	expression tag	UNP Q8A0E4
J	6	HIS	-	expression tag	UNP Q8A0E4
J	7	HIS	-	expression tag	UNP Q8A0E4
J	8	SER	-	expression tag	UNP Q8A0E4
J	9	SER	-	expression tag	UNP Q8A0E4
J	10	GLY	-	expression tag	UNP Q8A0E4
J	11	LEU	-	expression tag	UNP Q8A0E4
J	12	VAL	-	expression tag	UNP Q8A0E4
J	13	PRO	-	expression tag	UNP Q8A0E4
J	14	ARG	-	expression tag	UNP Q8A0E4
J	15	GLY	-	expression tag	UNP Q8A0E4
J	16	SER	-	expression tag	UNP Q8A0E4
J	17	HIS	-	expression tag	UNP Q8A0E4
J	18	MET	-	expression tag	UNP Q8A0E4
J	19	LEU	-	expression tag	UNP Q8A0E4
J	20	GLU	-	expression tag	UNP Q8A0E4
J	150	ALA	SER	engineered mutation	UNP Q8A0E4

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	1	0
2	B	1	Total Ca 1 1	1	0
2	C	1	Total Ca 1 1	1	0
2	D	1	Total Ca 1 1	1	0
2	E	1	Total Ca 1 1	1	0
2	F	1	Total Ca 1 1	1	0
2	G	1	Total Ca 1 1	1	0
2	H	1	Total Ca 1 1	1	0
2	I	2	Total Ca 2 2	2	0

- Molecule 3 is Trans-methylferulate (three-letter code: SZQ) (formula: $C_{11}H_{12}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 15 11 4	0	0
3	B	1	Total C O 15 11 4	0	0
3	E	1	Total C O 15 11 4	0	0
3	F	1	Total C O 15 11 4	0	0
3	G	1	Total C O 15 11 4	0	0
3	H	1	Total C O 15 11 4	0	0
3	I	1	Total C O 15 11 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	58	Total O 58 58	0	0
4	B	50	Total O 50 50	0	0
4	C	41	Total O 41 41	0	0

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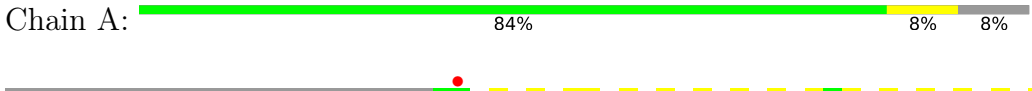
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	51	Total O 51 51	0	0
4	E	41	Total O 41 41	0	0
4	F	62	Total O 62 62	0	0
4	G	48	Total O 48 48	0	0
4	H	35	Total O 35 35	0	0
4	I	42	Total O 42 42	0	0
4	J	34	Total O 34 34	0	0

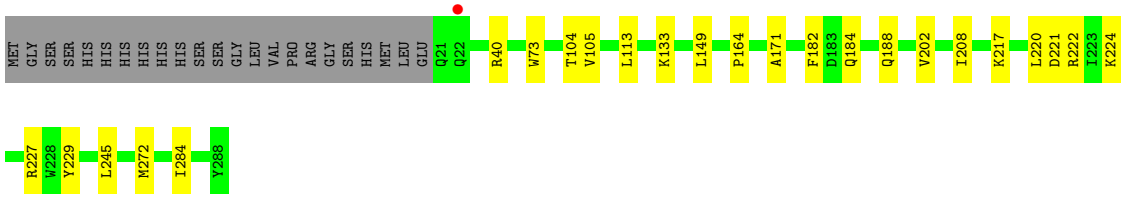
3 Residue-property plots (i)

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: Ferulic acid esterase

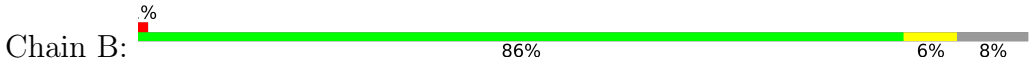
Chain A:

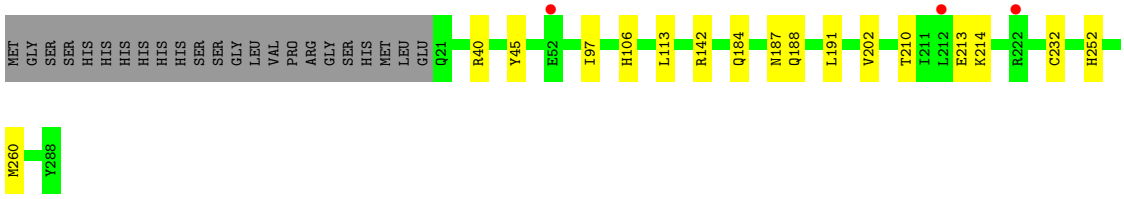




• Molecule 1: Ferulic acid esterase

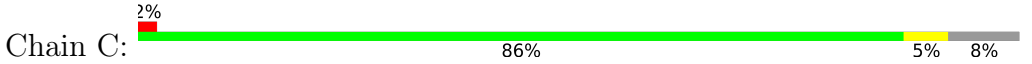
Chain B:

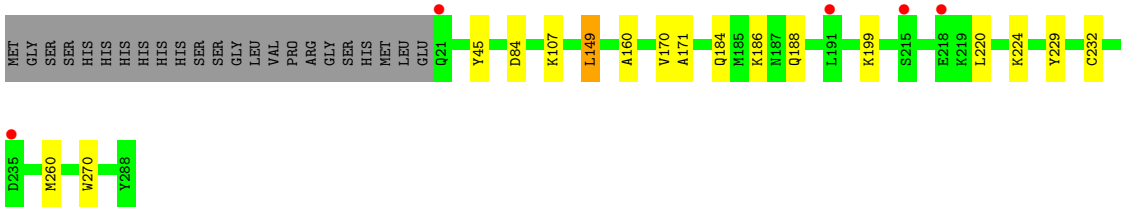




• Molecule 1: Ferulic acid esterase

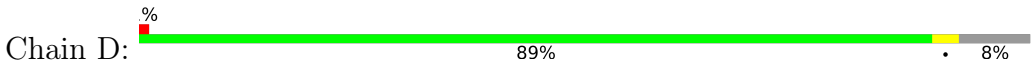
Chain C:

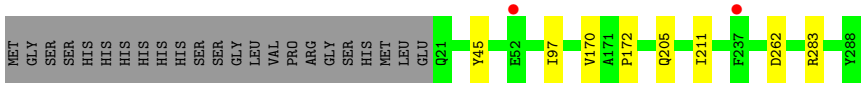




• Molecule 1: Ferulic acid esterase

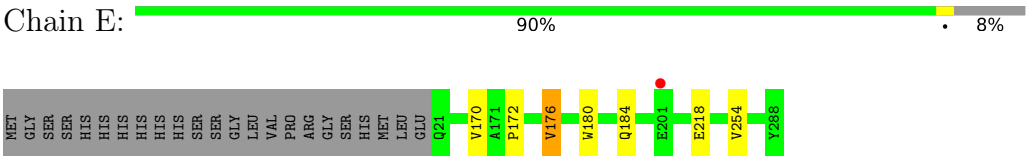
Chain D:





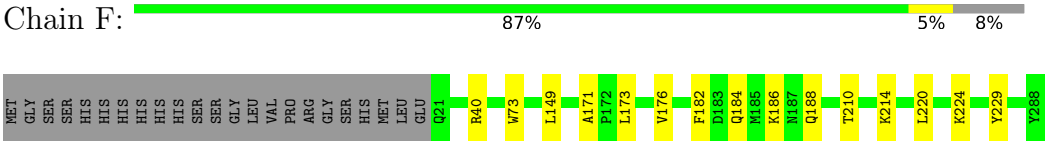
• Molecule 1: Ferulic acid esterase

Chain E:



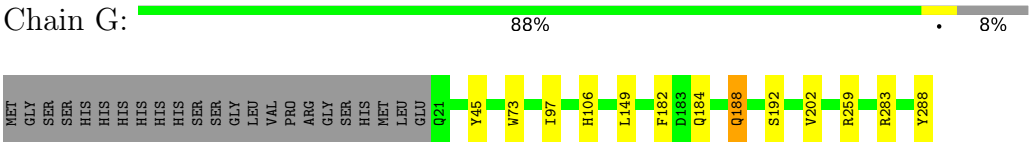
• Molecule 1: Ferulic acid esterase

Chain F:



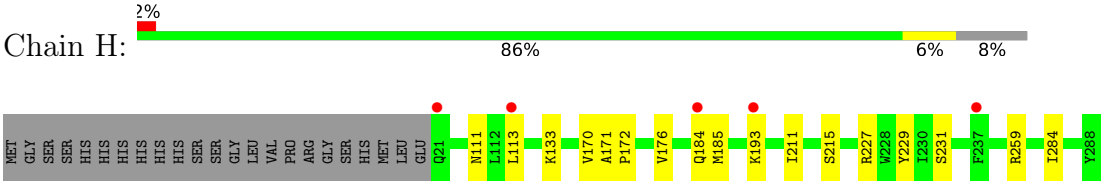
• Molecule 1: Ferulic acid esterase

Chain G:



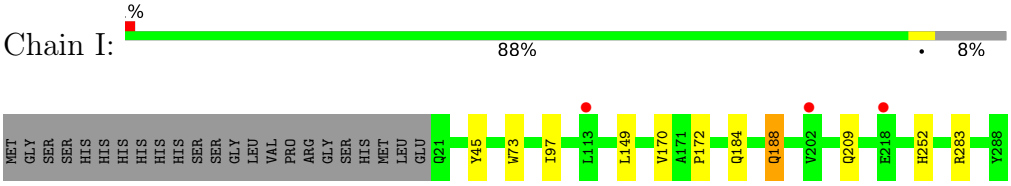
• Molecule 1: Ferulic acid esterase

Chain H:



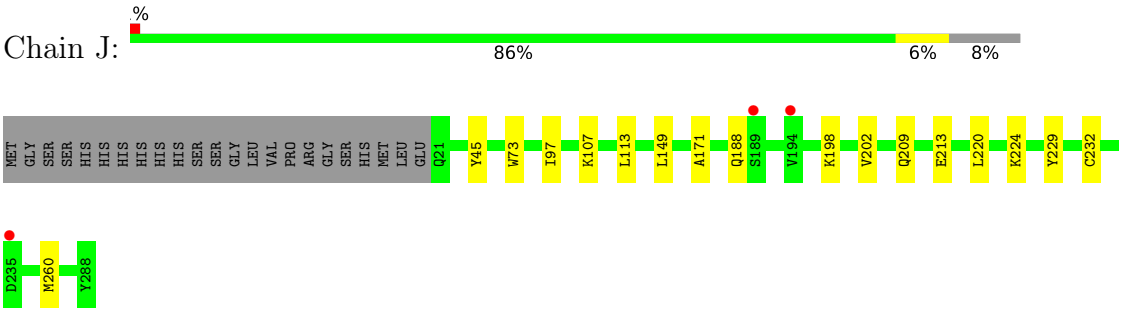
• Molecule 1: Ferulic acid esterase

Chain I:



• Molecule 1: Ferulic acid esterase

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	146.85Å 153.55Å 165.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.86 – 2.71 109.86 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.4 (109.86-2.71) 93.4 (109.86-2.71)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.179 , 0.228 0.179 , 0.228	Depositor DCC
R_{free} test set	1995 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22132	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: CA, SZQ

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	0.45	0/2218	0.61	0/3000
1	B	0.46	0/2225	0.60	0/3010
1	C	0.45	0/2218	0.61	0/2999
1	D	0.44	0/2209	0.59	0/2989
1	E	0.44	0/2218	0.60	0/3000
1	F	0.44	0/2210	0.60	0/2990
1	G	0.44	0/2210	0.61	0/2990
1	H	0.45	0/2210	0.62	0/2990
1	I	0.44	0/2210	0.58	0/2990
1	J	0.43	0/2210	0.59	0/2990
All	All	0.44	0/22138	0.60	0/29948

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2160	0	2090	16	0
1	B	2164	0	2097	10	0
1	C	2160	0	2093	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2151	0	2075	5	0
1	E	2160	0	2088	4	0
1	F	2152	0	2078	9	0
1	G	2152	0	2078	10	0
1	H	2152	0	2078	10	0
1	I	2152	0	2078	7	0
1	J	2152	0	2078	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	2	0	0	0	0
3	A	15	0	0	2	0
3	B	15	0	0	1	0
3	E	15	0	0	1	0
3	F	15	0	0	2	0
3	G	15	0	0	2	0
3	H	15	0	0	2	0
3	I	15	0	0	2	0
4	A	58	0	0	1	0
4	B	50	0	0	1	0
4	C	41	0	0	0	0
4	D	51	0	0	1	0
4	E	41	0	0	0	0
4	F	62	0	0	0	0
4	G	48	0	0	0	0
4	H	35	0	0	1	0
4	I	42	0	0	1	0
4	J	34	0	0	0	0
All	All	22132	0	20833	90	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 2.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HD11	1:A:202:VAL:HG21	1.52	0.90
1:B:210:THR:HG23	1:B:214:LYS:HE2	1.60	0.84
1:E:184:GLN:HG3	3:E:302:SZQ:C03	2.21	0.70
1:G:184:GLN:HG3	3:G:302:SZQ:C03	2.24	0.67
1:A:188:GLN:NE2	3:A:302:SZQ:O09	2.26	0.66
1:A:217:LYS:NZ	1:A:221:ASP:OD2	2.28	0.64
1:J:107:LYS:O	1:J:188:GLN:NE2	2.30	0.64
1:B:142:ARG:NH1	4:B:401:HOH:O	2.23	0.61
1:B:184:GLN:HG3	3:B:302:SZQ:C03	2.29	0.61
1:G:182:PHE:HE1	1:G:202:VAL:HG23	1.67	0.60
1:A:272:MET:SD	4:A:455:HOH:O	2.56	0.60
1:F:182:PHE:CE2	1:F:186:LYS:HD2	2.39	0.56
1:A:182:PHE:HE1	1:A:202:VAL:HG23	1.70	0.56
1:E:176:VAL:HG11	1:E:180:TRP:CE3	2.41	0.56
1:I:283:ARG:HD2	4:I:403:HOH:O	2.05	0.55
1:C:186:LYS:HD3	1:C:199:LYS:HE2	1.89	0.55
1:E:176:VAL:HG13	1:E:180:TRP:HB3	1.89	0.54
1:I:184:GLN:HG3	3:I:302:SZQ:C03	2.38	0.53
1:A:182:PHE:CE1	1:A:202:VAL:HG23	2.44	0.53
1:F:210:THR:HG23	1:F:214:LYS:HE2	1.90	0.53
1:I:188:GLN:NE2	3:I:302:SZQ:O09	2.37	0.53
1:F:184:GLN:HG3	3:F:302:SZQ:C03	2.39	0.52
1:J:198:LYS:O	1:J:202:VAL:HG23	2.10	0.51
1:C:149:LEU:HD13	1:C:270:TRP:CE3	2.46	0.51
1:G:106:HIS:CD2	1:G:188:GLN:HG3	2.45	0.51
1:D:283:ARG:HD2	4:D:402:HOH:O	2.11	0.50
1:C:107:LYS:O	1:C:188:GLN:NE2	2.44	0.50
1:G:188:GLN:NE2	3:G:302:SZQ:O09	2.34	0.50
1:H:170:VAL:HG12	1:H:172:PRO:HD3	1.94	0.49
1:B:113:LEU:HD21	1:B:202:VAL:HG11	1.94	0.49
1:I:209:GLN:OE1	1:I:252:HIS:CE1	2.66	0.48
1:G:106:HIS:HD2	1:G:188:GLN:HG3	1.77	0.48
1:A:104:THR:HG22	1:A:105:VAL:HG23	1.95	0.48
1:G:182:PHE:CE1	1:G:202:VAL:HG23	2.47	0.48
1:A:220:LEU:HG	1:A:224:LYS:HE3	1.96	0.47
1:A:227:ARG:HG3	1:A:284:ILE:HD12	1.95	0.47
1:F:73:TRP:CZ2	1:F:149:LEU:HD23	2.50	0.47
1:D:205:GLN:O	1:D:211:ILE:HD11	2.14	0.47
1:G:73:TRP:CZ2	1:G:149:LEU:HD23	2.49	0.47
1:H:193:LYS:HA	4:H:404:HOH:O	2.14	0.47
1:J:113:LEU:O	1:J:198:LYS:HE2	2.14	0.47
1:B:45:TYR:HB3	1:B:97:ILE:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:211:ILE:O	1:H:215:SER:OG	2.26	0.46
1:J:113:LEU:H	1:J:113:LEU:HD12	1.80	0.46
1:J:171:ALA:HA	1:J:229:TYR:O	2.16	0.45
1:F:188:GLN:NE2	3:F:302:SZQ:O09	2.48	0.45
1:J:73:TRP:CZ2	1:J:149:LEU:HD23	2.52	0.45
1:A:184:GLN:HG3	3:A:302:SZQ:C03	2.46	0.45
1:D:170:VAL:HG12	1:D:172:PRO:HD3	1.99	0.44
1:F:149:LEU:HA	1:F:173:LEU:O	2.17	0.44
1:A:164:PRO:HB2	1:A:222:ARG:HG3	2.00	0.44
1:H:227:ARG:HG3	1:H:284:ILE:HD12	2.00	0.44
1:J:209:GLN:O	1:J:213:GLU:HG3	2.17	0.44
1:B:232:CYS:O	1:B:260:MET:HA	2.18	0.44
1:C:232:CYS:O	1:C:260:MET:HA	2.18	0.43
1:C:220:LEU:HG	1:C:224:LYS:HE3	2.01	0.43
1:H:171:ALA:HA	1:H:229:TYR:O	2.18	0.43
1:J:220:LEU:HG	1:J:224:LYS:HE3	2.01	0.43
1:J:232:CYS:O	1:J:260:MET:HA	2.19	0.43
1:F:40:ARG:HA	1:F:40:ARG:HD2	1.74	0.43
1:C:171:ALA:HA	1:C:229:TYR:O	2.19	0.43
1:A:133:LYS:HE2	1:A:133:LYS:HB3	1.82	0.42
1:B:106:HIS:ND1	1:B:188:GLN:HG3	2.34	0.42
1:A:208:ILE:HD13	1:A:245:LEU:CD1	2.49	0.42
1:B:213:GLU:OE2	1:B:252:HIS:HE1	2.03	0.42
1:F:220:LEU:HG	1:F:224:LYS:HE3	2.01	0.42
1:E:170:VAL:HG12	1:E:172:PRO:HD3	2.02	0.42
1:H:111:ASN:O	1:H:185:MET:HE3	2.20	0.42
1:I:45:TYR:HB3	1:I:97:ILE:HB	2.02	0.42
1:J:45:TYR:HB3	1:J:97:ILE:HB	2.00	0.42
1:A:171:ALA:HA	1:A:229:TYR:O	2.19	0.42
1:C:107:LYS:HB2	1:C:188:GLN:HE22	1.85	0.42
1:A:73:TRP:CZ2	1:A:149:LEU:HD23	2.54	0.41
1:I:170:VAL:HG12	1:I:172:PRO:HD3	2.02	0.41
1:A:40:ARG:HD2	1:A:40:ARG:HA	1.91	0.41
1:G:45:TYR:HB3	1:G:97:ILE:HB	2.02	0.41
1:B:191:LEU:HD23	1:B:191:LEU:HA	1.89	0.41
1:C:160:ALA:CB	1:C:170:VAL:HG21	2.51	0.41
1:D:262:ASP:HB2	1:G:259:ARG:CZ	2.51	0.41
1:D:45:TYR:HB3	1:D:97:ILE:HB	2.03	0.41
1:F:171:ALA:HA	1:F:229:TYR:O	2.21	0.41
1:B:40:ARG:HD2	1:B:40:ARG:HA	1.90	0.41
1:C:45:TYR:OH	1:C:84:ASP:OD1	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:LEU:O	1:C:149:LEU:HG	2.20	0.41
1:G:283:ARG:HG2	1:G:288:TYR:CD2	2.56	0.41
1:H:184:GLN:HG3	3:H:302:SZQ:C02	2.51	0.41
1:I:73:TRP:CZ2	1:I:149:LEU:HD23	2.56	0.41
1:H:133:LYS:HE2	1:H:133:LYS:HB3	1.84	0.40
1:H:231:SER:HA	1:H:259:ARG:O	2.22	0.40
1:H:184:GLN:HG3	3:H:302:SZQ:C03	2.52	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	266/291 (91%)	260 (98%)	6 (2%)	0	100	100
1	B	267/291 (92%)	260 (97%)	7 (3%)	0	100	100
1	C	266/291 (91%)	259 (97%)	7 (3%)	0	100	100
1	D	266/291 (91%)	259 (97%)	7 (3%)	0	100	100
1	E	266/291 (91%)	258 (97%)	8 (3%)	0	100	100
1	F	266/291 (91%)	259 (97%)	7 (3%)	0	100	100
1	G	266/291 (91%)	259 (97%)	7 (3%)	0	100	100
1	H	266/291 (91%)	260 (98%)	6 (2%)	0	100	100
1	I	266/291 (91%)	259 (97%)	7 (3%)	0	100	100
1	J	266/291 (91%)	259 (97%)	7 (3%)	0	100	100
All	All	2661/2910 (91%)	2592 (97%)	69 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	227/249 (91%)	227 (100%)	0	100 100
1	B	228/249 (92%)	227 (100%)	1 (0%)	91 96
1	C	227/249 (91%)	225 (99%)	2 (1%)	78 91
1	D	224/249 (90%)	224 (100%)	0	100 100
1	E	227/249 (91%)	224 (99%)	3 (1%)	69 86
1	F	225/249 (90%)	224 (100%)	1 (0%)	91 96
1	G	225/249 (90%)	223 (99%)	2 (1%)	78 91
1	H	225/249 (90%)	223 (99%)	2 (1%)	78 91
1	I	225/249 (90%)	224 (100%)	1 (0%)	91 96
1	J	225/249 (90%)	225 (100%)	0	100 100
All	All	2258/2490 (91%)	2246 (100%)	12 (0%)	88 95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	187	ASN
1	C	149	LEU
1	C	184	GLN
1	E	176	VAL
1	E	218	GLU
1	E	254	VAL
1	F	176	VAL
1	G	188	GLN
1	G	192	SER
1	H	113	LEU
1	H	176	VAL
1	I	188	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	188	GLN
1	E	188	GLN
1	G	106	HIS
1	G	187	ASN
1	I	184	GLN
1	I	187	ASN
1	I	252	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 10 are monoatomic - leaving 7 for Mogul analysis.

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	SZQ	F	302	-	15,15,15	3.76	7 (46%)	19,19,19	2.97	7 (36%)
3	SZQ	H	302	-	15,15,15	3.57	8 (53%)	19,19,19	2.57	4 (21%)
3	SZQ	A	302	-	15,15,15	3.76	8 (53%)	19,19,19	2.33	4 (21%)
3	SZQ	B	302	-	15,15,15	3.71	8 (53%)	19,19,19	2.51	3 (15%)
3	SZQ	I	302	-	15,15,15	3.62	9 (60%)	19,19,19	2.58	4 (21%)
3	SZQ	E	302	-	15,15,15	3.87	11 (73%)	19,19,19	2.24	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SZQ	G	302	-	15,15,15	3.91	10 (66%)	19,19,19	2.55	6 (31%)

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	SZQ	F	302	-	-	5/9/9/9	0/1/1/1
3	SZQ	H	302	-	-	7/9/9/9	0/1/1/1
3	SZQ	A	302	-	-	7/9/9/9	0/1/1/1
3	SZQ	B	302	-	-	4/9/9/9	0/1/1/1
3	SZQ	I	302	-	-	7/9/9/9	0/1/1/1
3	SZQ	E	302	-	-	0/9/9/9	0/1/1/1
3	SZQ	G	302	-	-	5/9/9/9	0/1/1/1

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	302	SZQ	C08-C07	11.37	1.62	1.33
3	E	302	SZQ	C08-C07	11.32	1.62	1.33
3	B	302	SZQ	C08-C07	11.11	1.61	1.33
3	A	302	SZQ	C08-C07	11.06	1.61	1.33
3	H	302	SZQ	C08-C07	10.83	1.61	1.33
3	F	302	SZQ	C08-C07	10.81	1.61	1.33
3	I	302	SZQ	C08-C07	10.70	1.60	1.33
3	F	302	SZQ	C04-C05	-5.98	1.29	1.40
3	A	302	SZQ	C04-C05	-5.31	1.30	1.40
3	G	302	SZQ	C04-C05	-4.76	1.31	1.40
3	B	302	SZQ	C04-C05	-4.49	1.32	1.40
3	I	302	SZQ	C04-C05	-4.31	1.32	1.40
3	E	302	SZQ	C04-C05	-4.28	1.32	1.40
3	E	302	SZQ	C08-C10	3.76	1.57	1.48
3	H	302	SZQ	O11-C10	-3.76	1.13	1.21
3	F	302	SZQ	O11-C10	-3.75	1.13	1.21
3	G	302	SZQ	O11-C10	-3.71	1.13	1.21
3	A	302	SZQ	O11-C10	-3.70	1.13	1.21
3	I	302	SZQ	O11-C10	-3.64	1.14	1.21
3	H	302	SZQ	C04-C05	-3.58	1.33	1.40
3	E	302	SZQ	C06-C05	3.54	1.45	1.38
3	G	302	SZQ	C06-C05	3.53	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	302	SZQ	C08-C10	3.52	1.56	1.48
3	E	302	SZQ	O11-C10	-3.51	1.14	1.21
3	B	302	SZQ	O11-C10	-3.47	1.14	1.21
3	A	302	SZQ	C08-C10	3.28	1.55	1.48
3	B	302	SZQ	C08-C10	3.26	1.55	1.48
3	B	302	SZQ	C06-C05	3.11	1.44	1.38
3	F	302	SZQ	C06-C05	3.00	1.44	1.38
3	I	302	SZQ	C08-C10	2.94	1.55	1.48
3	H	302	SZQ	C08-C10	2.92	1.55	1.48
3	F	302	SZQ	C08-C10	2.87	1.54	1.48
3	E	302	SZQ	C01-C07	2.61	1.55	1.47
3	I	302	SZQ	C06-C05	2.58	1.43	1.38
3	I	302	SZQ	O09-C04	2.58	1.41	1.36
3	H	302	SZQ	O09-C04	2.56	1.41	1.36
3	H	302	SZQ	C06-C05	2.55	1.43	1.38
3	G	302	SZQ	C01-C07	2.54	1.54	1.47
3	F	302	SZQ	C02-C01	-2.51	1.34	1.39
3	I	302	SZQ	C02-C01	-2.50	1.34	1.39
3	A	302	SZQ	C06-C05	2.50	1.43	1.38
3	G	302	SZQ	O12-C10	2.42	1.40	1.34
3	E	302	SZQ	O12-C10	2.31	1.40	1.34
3	E	302	SZQ	O09-C04	2.28	1.41	1.36
3	A	302	SZQ	C01-C07	2.27	1.54	1.47
3	G	302	SZQ	C06-C01	2.26	1.43	1.39
3	G	302	SZQ	O13-C05	2.26	1.40	1.37
3	H	302	SZQ	C01-C07	2.26	1.54	1.47
3	E	302	SZQ	C06-C01	2.25	1.43	1.39
3	I	302	SZQ	C03-C04	2.19	1.43	1.39
3	F	302	SZQ	O12-C10	2.18	1.39	1.34
3	B	302	SZQ	C01-C07	2.16	1.53	1.47
3	A	302	SZQ	C03-C02	2.12	1.42	1.38
3	B	302	SZQ	O09-C04	2.10	1.40	1.36
3	G	302	SZQ	C02-C01	-2.10	1.35	1.39
3	H	302	SZQ	C03-C04	2.09	1.43	1.39
3	A	302	SZQ	C02-C01	-2.09	1.35	1.39
3	I	302	SZQ	C01-C07	2.08	1.53	1.47
3	B	302	SZQ	C02-C01	-2.07	1.35	1.39
3	E	302	SZQ	C03-C02	2.04	1.42	1.38
3	E	302	SZQ	C02-C01	-2.01	1.35	1.39

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	302	SZQ	C01-C07-C08	-7.61	109.50	126.91
3	H	302	SZQ	C01-C07-C08	-7.38	110.02	126.91
3	F	302	SZQ	C01-C07-C08	-7.18	110.47	126.91
3	F	302	SZQ	O12-C10-C08	6.66	122.03	111.38
3	I	302	SZQ	O12-C10-C08	6.62	121.96	111.38
3	E	302	SZQ	O12-C10-C08	6.32	121.49	111.38
3	G	302	SZQ	O12-C10-C08	6.20	121.30	111.38
3	G	302	SZQ	C01-C07-C08	-6.16	112.80	126.91
3	A	302	SZQ	O12-C10-C08	6.00	120.97	111.38
3	I	302	SZQ	C07-C08-C10	-5.92	104.22	122.26
3	A	302	SZQ	C01-C07-C08	-5.87	113.48	126.91
3	F	302	SZQ	C07-C08-C10	-5.78	104.64	122.26
3	B	302	SZQ	O12-C10-C08	5.64	120.41	111.38
3	H	302	SZQ	O12-C10-C08	5.55	120.25	111.38
3	E	302	SZQ	C01-C07-C08	-5.46	114.42	126.91
3	I	302	SZQ	C01-C07-C08	-5.06	115.33	126.91
3	H	302	SZQ	C07-C08-C10	-3.89	110.42	122.26
3	B	302	SZQ	C07-C08-C10	-3.67	111.09	122.26
3	A	302	SZQ	C07-C08-C10	-3.66	111.12	122.26
3	E	302	SZQ	C07-C08-C10	-3.15	112.66	122.26
3	H	302	SZQ	O13-C05-C04	3.15	119.13	114.57
3	G	302	SZQ	C07-C08-C10	-3.09	112.86	122.26
3	F	302	SZQ	O09-C04-C05	-2.76	113.66	120.09
3	F	302	SZQ	C03-C02-C01	-2.68	117.75	121.25
3	I	302	SZQ	O13-C05-C04	2.63	118.38	114.57
3	A	302	SZQ	O13-C05-C04	2.51	118.21	114.57
3	G	302	SZQ	C14-O13-C05	2.45	121.23	117.53
3	G	302	SZQ	C06-C05-C04	-2.44	117.43	120.06
3	G	302	SZQ	C15-O12-C10	2.38	120.21	115.93
3	F	302	SZQ	O11-C10-C08	-2.17	115.98	123.58
3	F	302	SZQ	C03-C04-C05	2.13	122.00	119.53

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	SZQ	C01-C07-C08-C10
3	A	302	SZQ	C08-C10-O12-C15
3	F	302	SZQ	C01-C07-C08-C10
3	G	302	SZQ	C01-C07-C08-C10
3	G	302	SZQ	C08-C10-O12-C15
3	H	302	SZQ	C01-C07-C08-C10
3	I	302	SZQ	C01-C07-C08-C10

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Mol	Chain	Res	Type	Atoms
3	I	302	SZQ	C08-C10-O12-C15
3	H	302	SZQ	C08-C10-O12-C15
3	I	302	SZQ	O11-C10-O12-C15
3	A	302	SZQ	C04-C05-O13-C14
3	A	302	SZQ	O11-C10-O12-C15
3	H	302	SZQ	O11-C10-O12-C15
3	G	302	SZQ	O11-C10-O12-C15
3	F	302	SZQ	C04-C05-O13-C14
3	A	302	SZQ	C06-C05-O13-C14
3	F	302	SZQ	C06-C05-O13-C14
3	B	302	SZQ	C08-C10-O12-C15
3	I	302	SZQ	C04-C05-O13-C14
3	G	302	SZQ	C07-C08-C10-O12
3	B	302	SZQ	O11-C10-O12-C15
3	G	302	SZQ	C07-C08-C10-O11
3	I	302	SZQ	C06-C05-O13-C14
3	I	302	SZQ	C07-C08-C10-O12
3	I	302	SZQ	C07-C08-C10-O11
3	H	302	SZQ	C06-C01-C07-C08
3	F	302	SZQ	C07-C08-C10-O12
3	H	302	SZQ	C02-C01-C07-C08
3	B	302	SZQ	C07-C08-C10-O12
3	A	302	SZQ	C07-C08-C10-O12
3	H	302	SZQ	C07-C08-C10-O12
3	B	302	SZQ	C07-C08-C10-O11
3	F	302	SZQ	C07-C08-C10-O11
3	A	302	SZQ	C07-C08-C10-O11
3	H	302	SZQ	C07-C08-C10-O11

There are no ring outliers.

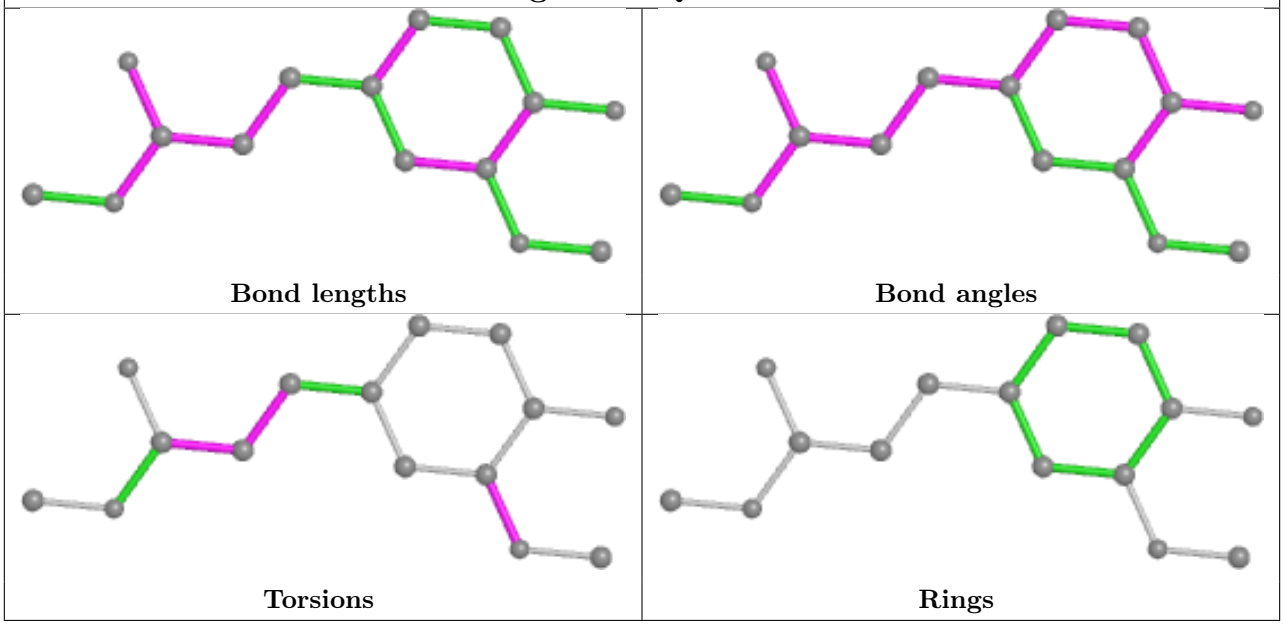
7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	302	SZQ	2	0
3	H	302	SZQ	2	0
3	A	302	SZQ	2	0
3	B	302	SZQ	1	0
3	I	302	SZQ	2	0
3	E	302	SZQ	1	0
3	G	302	SZQ	2	0

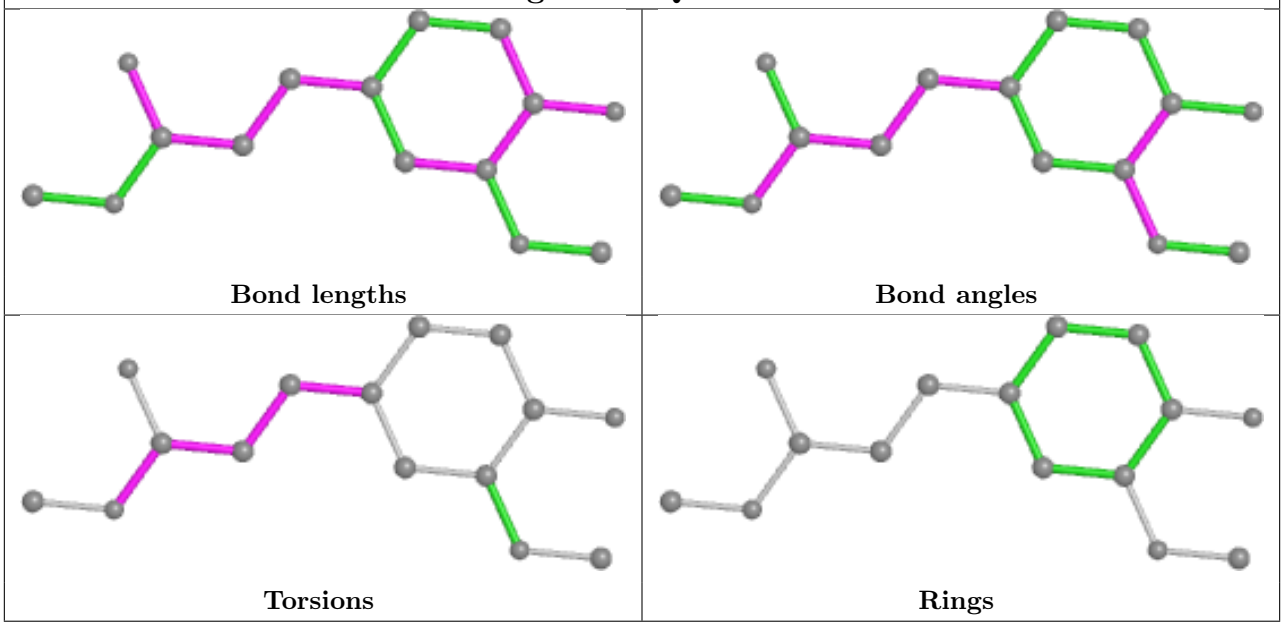
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

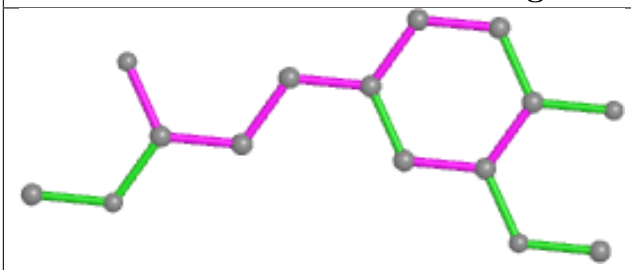
Ligand SZQ F 302



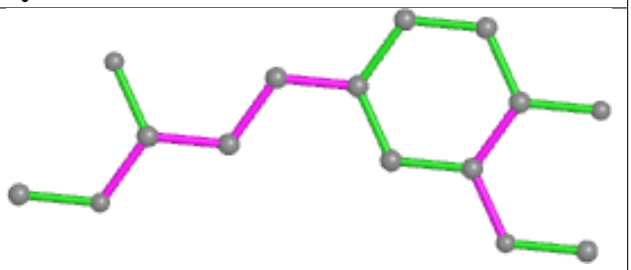
Ligand SZQ H 302



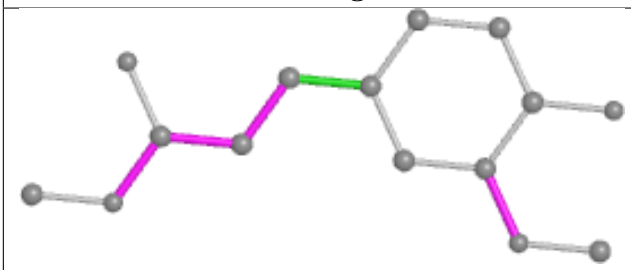
Ligand SZQ A 302



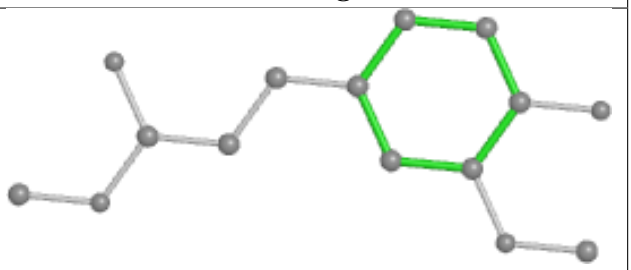
Bond lengths



Bond angles

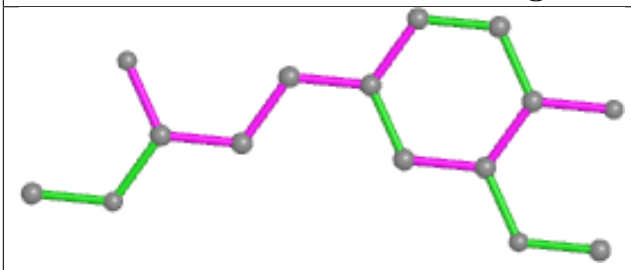


Torsions

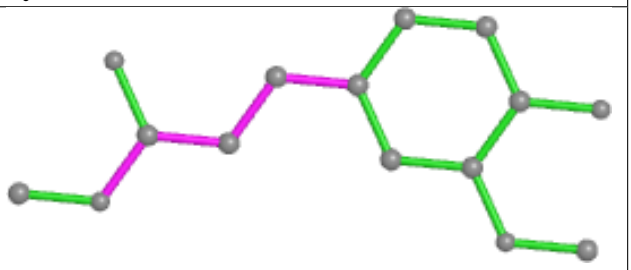


Rings

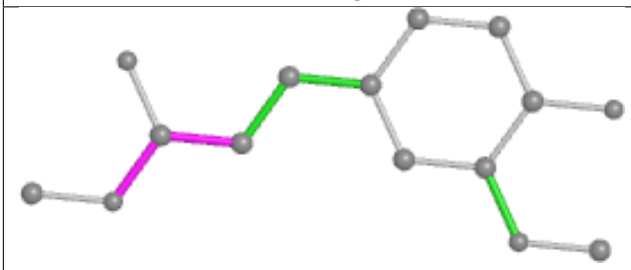
Ligand SZQ B 302



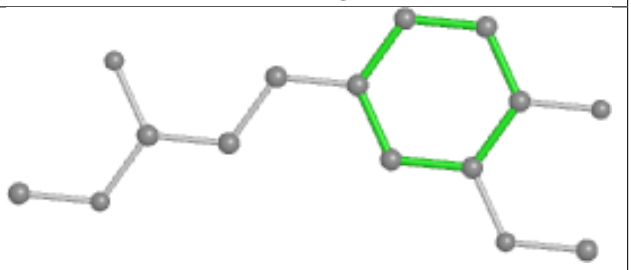
Bond lengths



Bond angles

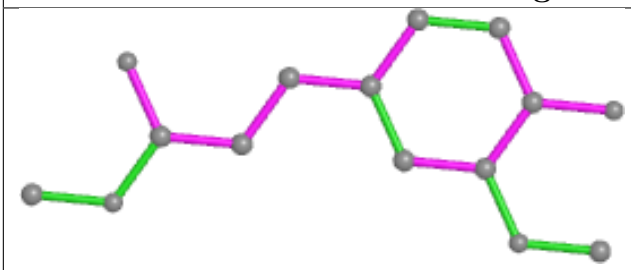


Torsions

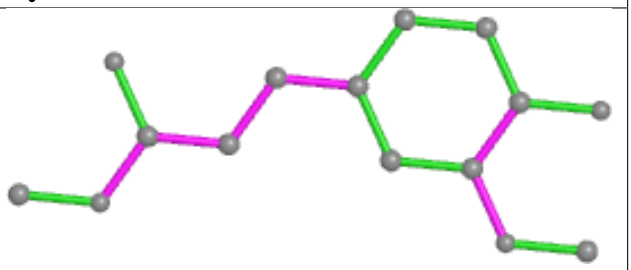


Rings

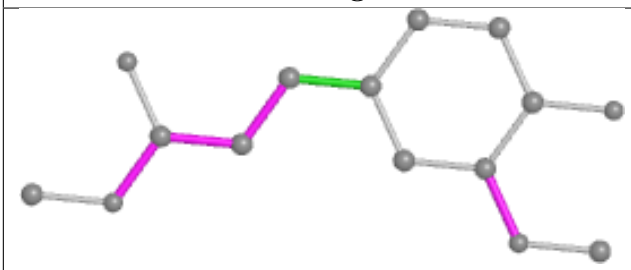
Ligand SZQ I 302



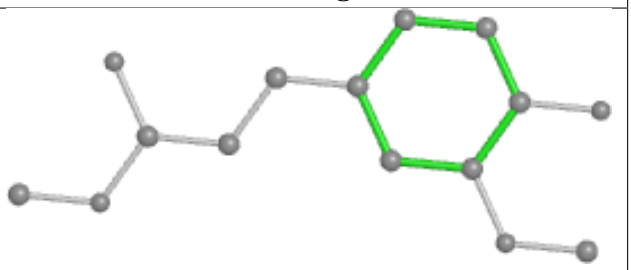
Bond lengths



Bond angles

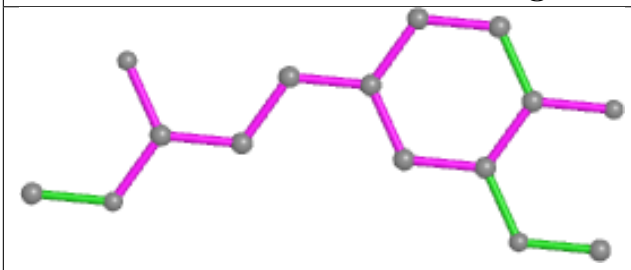


Torsions

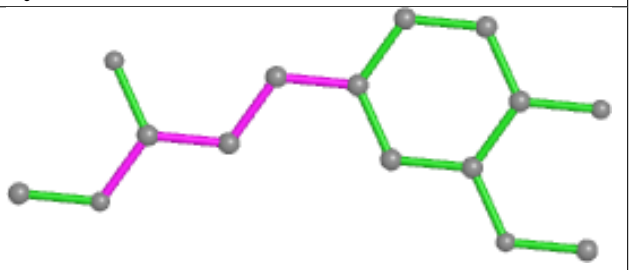


Rings

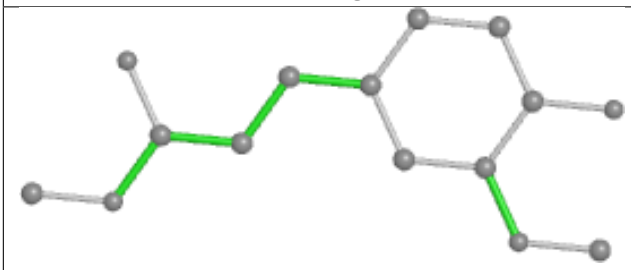
Ligand SZQ E 302



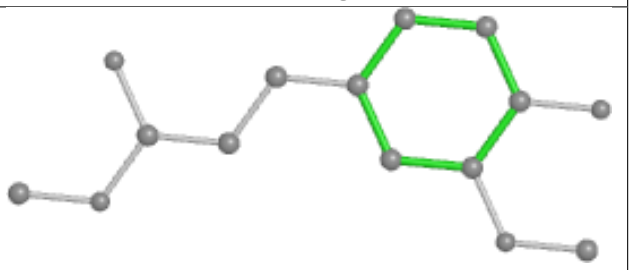
Bond lengths



Bond angles

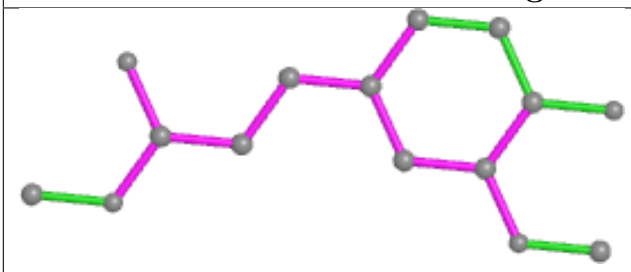


Torsions

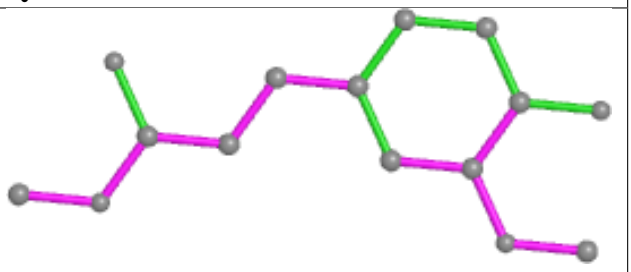


Rings

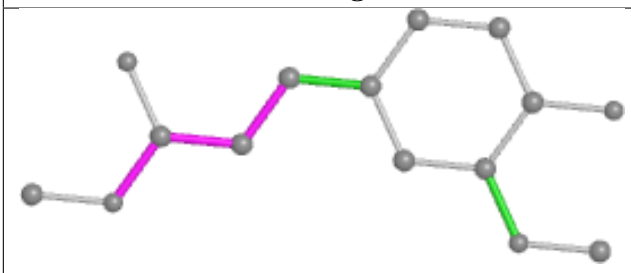
Ligand SZQ G 302



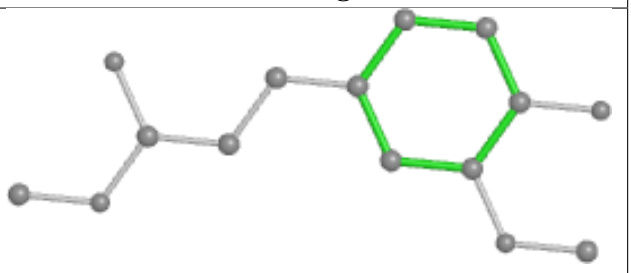
Bond lengths



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	268/291 (92%)	0.13	1 (0%) 92 93	24, 37, 65, 83	0
1	B	268/291 (92%)	0.22	3 (1%) 80 82	26, 41, 74, 106	0
1	C	268/291 (92%)	0.24	5 (1%) 66 69	27, 41, 71, 93	0
1	D	268/291 (92%)	0.10	2 (0%) 87 89	26, 39, 57, 94	0
1	E	268/291 (92%)	0.12	1 (0%) 92 93	25, 40, 71, 95	0
1	F	268/291 (92%)	0.05	0 100 100	25, 39, 62, 90	0
1	G	268/291 (92%)	0.10	0 100 100	26, 41, 75, 104	0
1	H	268/291 (92%)	0.27	5 (1%) 66 69	26, 41, 74, 116	0
1	I	268/291 (92%)	0.19	3 (1%) 80 82	28, 42, 74, 106	0
1	J	268/291 (92%)	0.22	3 (1%) 80 82	27, 41, 76, 99	0
All	All	2680/2910 (92%)	0.16	23 (0%) 84 85	24, 40, 72, 116	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	113	LEU	4.1
1	C	191	LEU	3.7
1	C	21	GLN	3.4
1	D	237	PHE	3.2
1	I	202	VAL	3.0
1	A	22	GLN	2.8
1	H	193	LYS	2.8
1	D	52	GLU	2.7
1	B	52	GLU	2.6
1	J	189	SER	2.6
1	J	235	ASP	2.4
1	C	215	SER	2.4
1	C	235	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	194	VAL	2.3
1	H	184	GLN	2.2
1	B	222	ARG	2.2
1	C	218	GLU	2.2
1	H	21	GLN	2.2
1	E	201	GLU	2.1
1	B	212	LEU	2.1
1	H	237	PHE	2.0
1	I	218	GLU	2.0
1	I	113	LEU	2.0

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)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.