Full wwPDB X-ray Structure Validation Report ⓘ

Mar 11, 2024 – 11:34 AM EDT

PDB ID	:	8GKF
Title	:	Phosphopantetheinyl transferase PptT from Mycobacterium tuberculosis in complex with Raltitrexed.
Authors	:	Krieger, I.V.; Singh, A.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on	:	2023-03-18
Resolution	:	2.45 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:

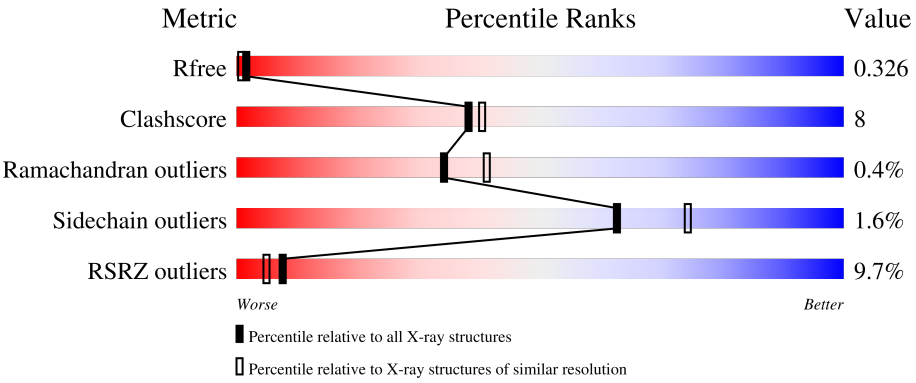
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	235	3% 82% 11% 6%
1	B	235	5% 83% 12% 5%
1	C	235	6% 77% 18% • •
1	D	235	9% 83% 12% • •

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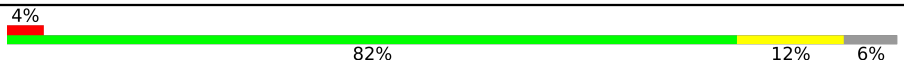
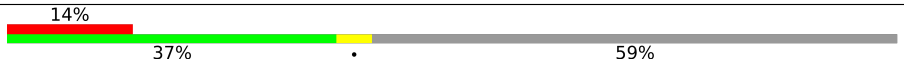
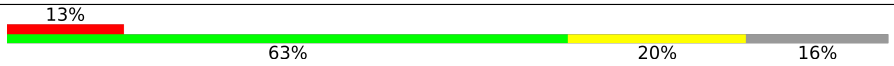
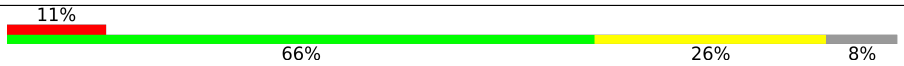
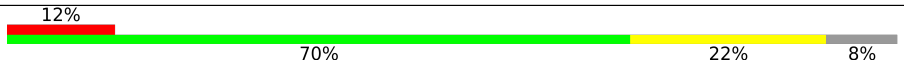
Mol	Chain	Length	Quality of chain
1	E	235	
1	F	235	
1	G	235	
1	H	235	
1	I	235	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14268 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 4'-phosphopantetheinyl transferase PptT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1686	1077	299	303	7			
1	B	223	Total	C	N	O	S	0	0	0
			1708	1093	302	306	7			
1	C	225	Total	C	N	O	S	0	0	0
			1712	1093	301	311	7			
1	D	225	Total	C	N	O	S	0	0	0
			1659	1061	296	297	5			
1	E	222	Total	C	N	O	S	0	0	0
			1672	1072	295	298	7			
1	F	97	Total	C	N	O	S	0	0	0
			701	455	121	123	2			
1	G	197	Total	C	N	O	S	0	0	0
			1508	968	267	268	5			
1	H	216	Total	C	N	O	S	0	0	0
			1617	1039	279	293	6			
1	I	217	Total	C	N	O	S	0	0	0
			1642	1049	284	302	7			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	ALA	-	expression tag	UNP O33336
A	229	GLY	-	expression tag	UNP O33336
A	230	GLU	-	expression tag	UNP O33336
A	231	ASN	-	expression tag	UNP O33336
A	232	LEU	-	expression tag	UNP O33336
A	233	TYR	-	expression tag	UNP O33336
A	234	PHE	-	expression tag	UNP O33336
A	235	GLN	-	expression tag	UNP O33336
B	228	ALA	-	expression tag	UNP O33336
B	229	GLY	-	expression tag	UNP O33336
B	230	GLU	-	expression tag	UNP O33336

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Chain	Residue	Modelled	Actual	Comment	Reference
B	231	ASN	-	expression tag	UNP O33336
B	232	LEU	-	expression tag	UNP O33336
B	233	TYR	-	expression tag	UNP O33336
B	234	PHE	-	expression tag	UNP O33336
B	235	GLN	-	expression tag	UNP O33336
C	228	ALA	-	expression tag	UNP O33336
C	229	GLY	-	expression tag	UNP O33336
C	230	GLU	-	expression tag	UNP O33336
C	231	ASN	-	expression tag	UNP O33336
C	232	LEU	-	expression tag	UNP O33336
C	233	TYR	-	expression tag	UNP O33336
C	234	PHE	-	expression tag	UNP O33336
C	235	GLN	-	expression tag	UNP O33336
D	228	ALA	-	expression tag	UNP O33336
D	229	GLY	-	expression tag	UNP O33336
D	230	GLU	-	expression tag	UNP O33336
D	231	ASN	-	expression tag	UNP O33336
D	232	LEU	-	expression tag	UNP O33336
D	233	TYR	-	expression tag	UNP O33336
D	234	PHE	-	expression tag	UNP O33336
D	235	GLN	-	expression tag	UNP O33336
E	228	ALA	-	expression tag	UNP O33336
E	229	GLY	-	expression tag	UNP O33336
E	230	GLU	-	expression tag	UNP O33336
E	231	ASN	-	expression tag	UNP O33336
E	232	LEU	-	expression tag	UNP O33336
E	233	TYR	-	expression tag	UNP O33336
E	234	PHE	-	expression tag	UNP O33336
E	235	GLN	-	expression tag	UNP O33336
F	228	ALA	-	expression tag	UNP O33336
F	229	GLY	-	expression tag	UNP O33336
F	230	GLU	-	expression tag	UNP O33336
F	231	ASN	-	expression tag	UNP O33336
F	232	LEU	-	expression tag	UNP O33336
F	233	TYR	-	expression tag	UNP O33336
F	234	PHE	-	expression tag	UNP O33336
F	235	GLN	-	expression tag	UNP O33336
G	228	ALA	-	expression tag	UNP O33336
G	229	GLY	-	expression tag	UNP O33336
G	230	GLU	-	expression tag	UNP O33336
G	231	ASN	-	expression tag	UNP O33336
G	232	LEU	-	expression tag	UNP O33336

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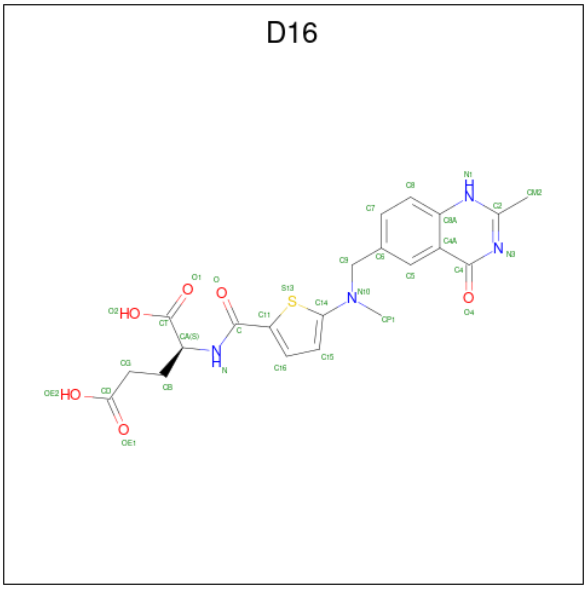
Chain	Residue	Modelled	Actual	Comment	Reference
G	233	TYR	-	expression tag	UNP O33336
G	234	PHE	-	expression tag	UNP O33336
G	235	GLN	-	expression tag	UNP O33336
H	228	ALA	-	expression tag	UNP O33336
H	229	GLY	-	expression tag	UNP O33336
H	230	GLU	-	expression tag	UNP O33336
H	231	ASN	-	expression tag	UNP O33336
H	232	LEU	-	expression tag	UNP O33336
H	233	TYR	-	expression tag	UNP O33336
H	234	PHE	-	expression tag	UNP O33336
H	235	GLN	-	expression tag	UNP O33336
I	228	ALA	-	expression tag	UNP O33336
I	229	GLY	-	expression tag	UNP O33336
I	230	GLU	-	expression tag	UNP O33336
I	231	ASN	-	expression tag	UNP O33336
I	232	LEU	-	expression tag	UNP O33336
I	233	TYR	-	expression tag	UNP O33336
I	234	PHE	-	expression tag	UNP O33336
I	235	GLN	-	expression tag	UNP O33336

- Molecule 2 is TOMUDEX (three-letter code: D16) (formula: $C_{21}H_{22}N_4O_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			32	21	4	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	C	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	D	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	E	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	F	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	G	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	H	1	Total	C	N	O	S	0	0
			32	21	4	6	1		
2	I	1	Total	C	N	O	S	0	0
			32	21	4	6	1		

- Molecule 3 is water.

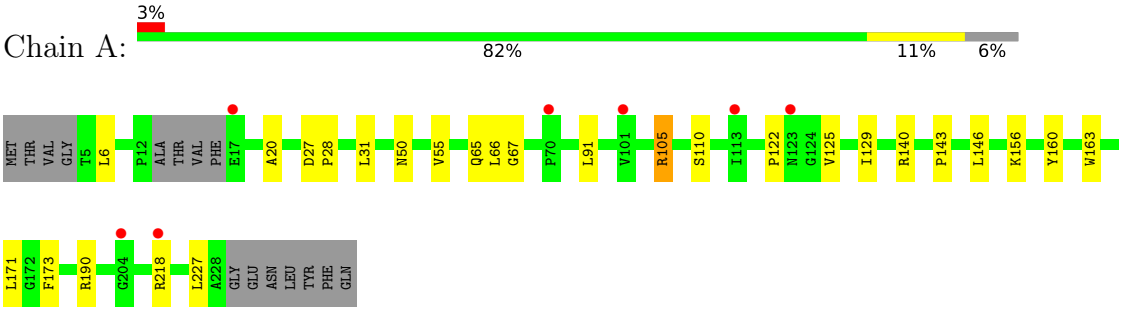
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	20	Total	O	0	0
			20	20		
3	C	6	Total	O	0	0
			6	6		
3	D	7	Total	O	0	0
			7	7		
3	E	8	Total	O	0	0
			8	8		
3	F	3	Total	O	0	0
			3	3		
3	G	9	Total	O	0	0
			9	9		
3	H	10	Total	O	0	0
			10	10		
3	I	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

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

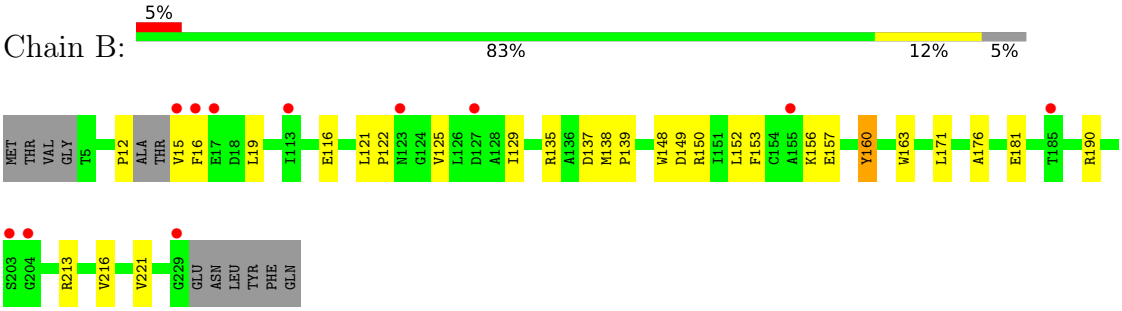
• Molecule 1: 4'-phosphopantetheinyl transferase PptT

Chain A:



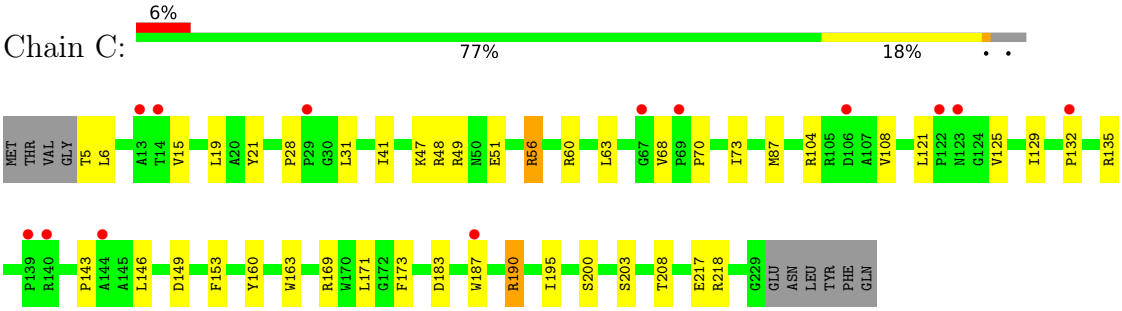
• Molecule 1: 4'-phosphopantetheinyl transferase PptT

Chain B:



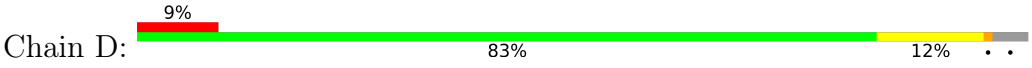
• Molecule 1: 4'-phosphopantetheinyl transferase PptT

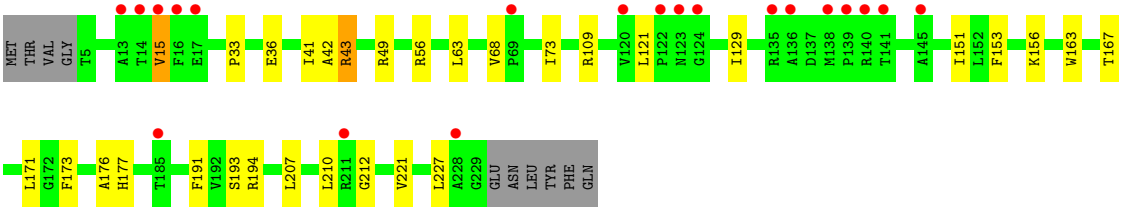
Chain C:



• Molecule 1: 4'-phosphopantetheinyl transferase PptT

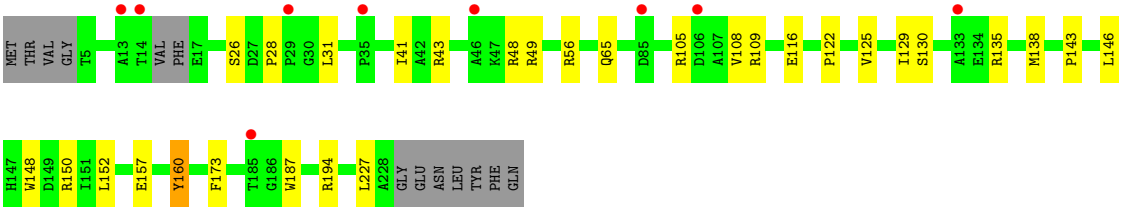
Chain D:





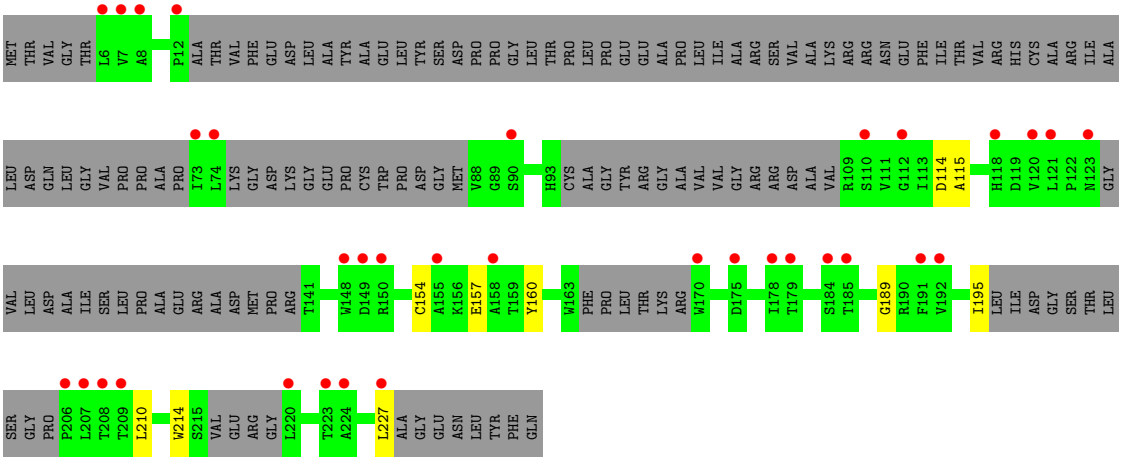
• Molecule 1: 4'-phosphopantetheinyl transferase PptT

Chain E:



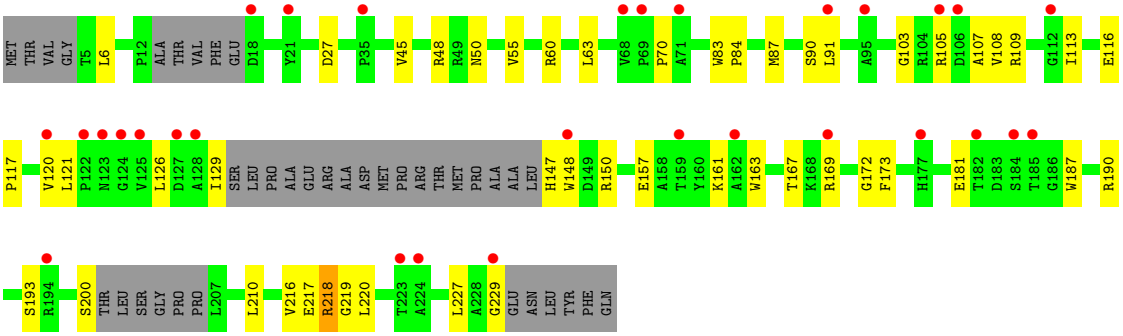
• Molecule 1: 4'-phosphopantetheinyl transferase PptT

Chain F:



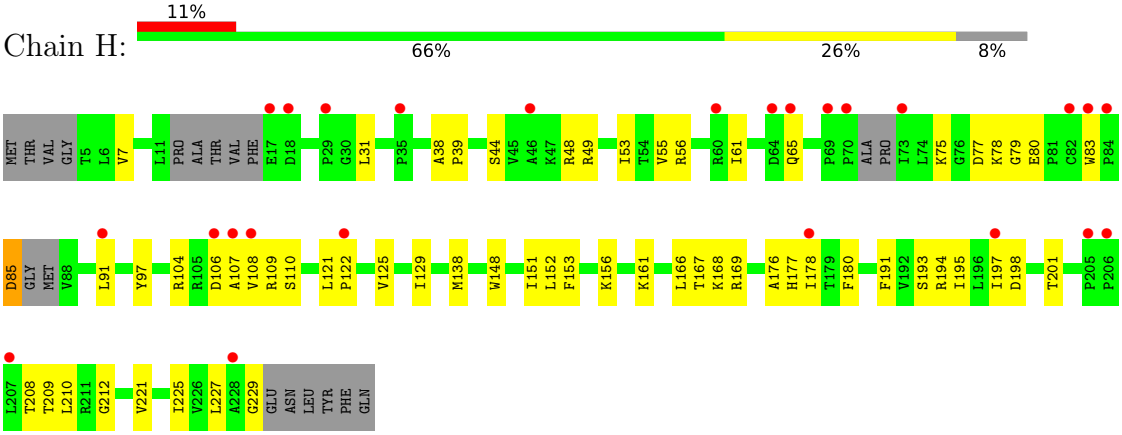
• Molecule 1: 4'-phosphopantetheinyl transferase PptT

Chain G:



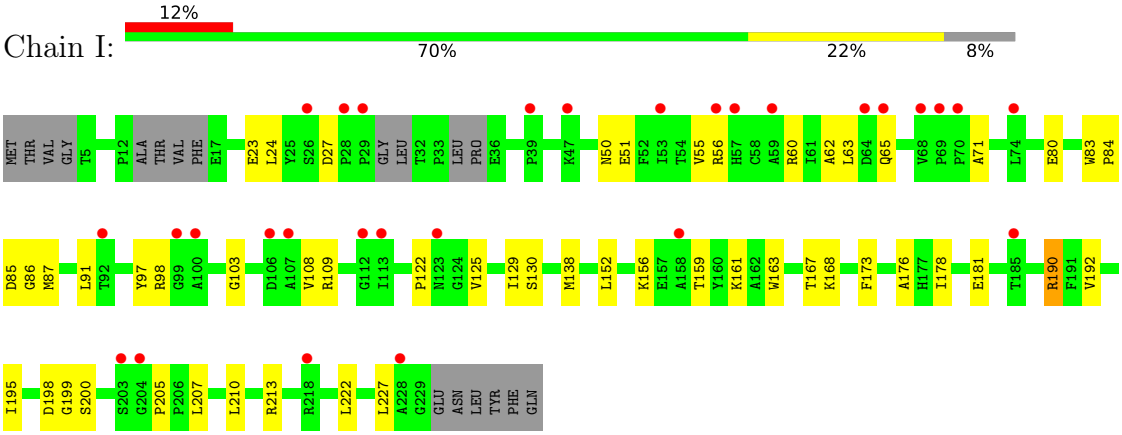
• Molecule 1: 4'-phosphopantetheinyl transferase PptT

Chain H:



• Molecule 1: 4'-phosphopantetheinyl transferase PptT

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	141.83Å 141.83Å 209.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.08 – 2.45 21.35 – 2.45	Depositor EDS
% Data completeness (in resolution range)	91.0 (21.08-2.45) 91.0 (21.35-2.45)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.44Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.281 , 0.326 0.282 , 0.326	Depositor DCC
R_{free} test set	3605 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	14268	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4281e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: D16

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	0.31	0/1730	0.53	0/2363
1	B	0.34	0/1753	0.58	0/2394
1	C	0.33	0/1757	0.58	0/2403
1	D	0.36	0/1702	0.61	0/2330
1	E	0.39	0/1716	0.56	0/2348
1	F	0.28	0/712	0.62	0/965
1	G	0.40	0/1545	0.63	0/2106
1	H	0.38	0/1657	0.64	0/2264
1	I	0.37	0/1683	0.62	0/2299
All	All	0.36	0/14255	0.59	0/19472

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	1686	0	1695	18	0
1	B	1708	0	1716	20	0
1	C	1712	0	1715	28	0
1	D	1659	0	1628	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1672	0	1673	18	0
1	F	701	0	653	6	0
1	G	1508	0	1508	37	0
1	H	1617	0	1586	41	0
1	I	1642	0	1622	29	0
2	A	32	0	20	0	0
2	B	32	0	20	0	0
2	C	32	0	20	2	0
2	D	32	0	20	0	0
2	E	32	0	20	2	0
2	F	32	0	20	0	0
2	G	32	0	20	2	0
2	H	32	0	20	2	0
2	I	32	0	20	0	0
3	A	11	0	0	0	0
3	B	20	0	0	0	0
3	C	6	0	0	0	0
3	D	7	0	0	0	0
3	E	8	0	0	0	0
3	F	3	0	0	0	0
3	G	9	0	0	0	0
3	H	10	0	0	0	0
3	I	1	0	0	0	0
All	All	14268	0	13976	213	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 8.

All (213) 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:G:169:ARG:HH22	1:G:200:SER:HB2	1.27	0.98
1:G:169:ARG:NH2	1:G:200:SER:HB2	1.95	0.81
1:A:122:PRO:HG2	1:A:125:VAL:HG21	1.66	0.76
1:G:181:GLU:HG3	1:G:190:ARG:HE	1.50	0.75
1:H:167:THR:HB	1:H:201:THR:HA	1.69	0.73
1:H:152:LEU:HD11	1:H:156:LYS:HE2	1.70	0.72
1:I:80:GLU:OE2	1:I:168:LYS:NZ	2.21	0.70
1:B:156:LYS:NZ	1:B:176:ALA:O	2.25	0.69
1:E:157:GLU:HG2	1:E:160:TYR:CE2	2.28	0.69
1:A:20:ALA:HB1	1:A:65:GLN:HE21	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:PRO:HG2	1:B:125:VAL:HG21	1.75	0.67
1:G:109:ARG:N	1:G:227:LEU:O	2.28	0.67
1:G:181:GLU:CG	1:G:190:ARG:HE	2.08	0.66
1:H:106:ASP:OD1	1:H:107:ALA:N	2.28	0.66
1:I:156:LYS:NZ	1:I:176:ALA:O	2.27	0.65
1:B:139:PRO:O	1:C:218:ARG:HD2	1.97	0.65
1:H:75:LYS:HD3	2:H:301:D16:OE1	1.97	0.65
1:B:129:ILE:HG21	1:B:153:PHE:HD1	1.62	0.64
1:G:187:TRP:HB3	1:G:216:VAL:HG22	1.80	0.64
1:C:56:ARG:HG2	1:C:73:ILE:HD12	1.80	0.63
1:I:198:ASP:OD1	1:I:200:SER:N	2.25	0.63
1:I:103:GLY:HA3	1:I:108:VAL:HG21	1.80	0.63
1:H:77:ASP:C	1:H:79:GLY:H	2.03	0.62
1:B:12:PRO:HB2	1:B:15:VAL:HG21	1.81	0.62
1:G:6:LEU:HD22	1:G:217:GLU:HB3	1.83	0.61
1:B:157:GLU:HB2	1:B:160:TYR:CE2	2.35	0.61
1:I:91:LEU:O	1:I:161:LYS:NZ	2.29	0.61
1:D:193:SER:HB2	1:D:210:LEU:HB2	1.82	0.60
1:G:120:VAL:HG13	1:G:147:HIS:CE1	2.36	0.60
1:H:193:SER:HB2	1:H:210:LEU:HB2	1.84	0.60
1:I:122:PRO:HG2	1:I:125:VAL:HG21	1.83	0.60
1:G:157:GLU:HG2	1:G:161:LYS:HD2	1.84	0.59
1:D:210:LEU:HD12	1:D:227:LEU:HD21	1.85	0.58
1:I:109:ARG:N	1:I:227:LEU:O	2.34	0.58
1:B:139:PRO:HG3	1:B:148:TRP:CE2	2.38	0.58
1:C:6:LEU:HD22	1:C:217:GLU:HG2	1.87	0.57
1:I:55:VAL:HG11	1:I:91:LEU:HB3	1.87	0.57
1:H:210:LEU:HD13	1:H:227:LEU:HD21	1.87	0.57
1:A:105:ARG:HB2	1:A:105:ARG:HH11	1.70	0.56
1:C:121:LEU:HD13	1:C:125:VAL:HG23	1.86	0.56
1:G:90:SER:HB3	1:G:113:ILE:HG12	1.87	0.56
1:D:56:ARG:HG2	1:D:73:ILE:HD12	1.87	0.56
1:H:129:ILE:HG21	1:H:153:PHE:HD1	1.70	0.56
1:D:129:ILE:HA	1:D:173:PHE:HB3	1.88	0.56
1:G:161:LYS:NZ	2:G:301:D16:O	2.39	0.56
1:B:129:ILE:HG21	1:B:153:PHE:CD1	2.39	0.56
1:E:157:GLU:HG2	1:E:160:TYR:CZ	2.42	0.55
1:B:181:GLU:OE1	1:B:190:ARG:NH2	2.38	0.55
1:C:87:MET:HE2	1:C:104:ARG:HA	1.87	0.55
1:H:177:HIS:O	1:H:194:ARG:N	2.40	0.55
1:I:60:ARG:HA	1:I:63:LEU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:210:LEU:HD23	1:I:227:LEU:HD21	1.89	0.55
1:C:5:THR:HG1	1:C:21:TYR:HE2	1.55	0.55
1:H:56:ARG:HH12	2:H:301:D16:CD	2.20	0.54
1:I:207:LEU:HD21	1:I:210:LEU:HD21	1.90	0.54
1:C:47:LYS:NZ	1:C:51:GLU:OE2	2.29	0.54
1:H:107:ALA:O	1:H:229:GLY:N	2.34	0.54
1:E:129:ILE:HA	1:E:173:PHE:HB3	1.90	0.54
1:G:172:GLY:HA2	2:G:301:D16:HM21	1.88	0.54
1:E:135:ARG:HG3	1:E:148:TRP:HH2	1.73	0.54
1:G:103:GLY:HA3	1:G:108:VAL:HG21	1.89	0.54
1:B:138:MET:SD	1:B:152:LEU:HB2	2.49	0.53
1:C:183:ASP:OD1	1:C:190:ARG:NH1	2.42	0.53
1:I:23:GLU:O	1:I:24:LEU:HD12	2.08	0.53
1:H:210:LEU:HD12	1:H:225:ILE:HG21	1.89	0.53
1:A:163:TRP:CD1	1:A:171:LEU:HB2	2.45	0.52
1:C:169:ARG:NH2	1:C:200:SER:O	2.43	0.52
1:D:156:LYS:NZ	1:D:176:ALA:O	2.37	0.52
1:B:216:VAL:HG22	1:B:221:VAL:HG22	1.92	0.52
1:C:121:LEU:HB3	1:C:125:VAL:CG2	2.40	0.52
1:H:85:ASP:OD1	1:H:85:ASP:N	2.42	0.52
1:I:62:ALA:HA	1:I:65:GLN:OE1	2.11	0.51
1:C:63:LEU:HD22	1:C:68:VAL:HG11	1.92	0.51
1:H:178:ILE:HG23	1:H:180:PHE:HE1	1.74	0.51
1:G:121:LEU:HA	1:G:150:ARG:HH21	1.75	0.51
1:D:163:TRP:CE3	1:D:171:LEU:HB2	2.45	0.51
1:G:60:ARG:HD3	1:G:70:PRO:HB3	1.91	0.51
1:E:56:ARG:HH12	2:E:301:D16:CD	2.24	0.51
1:F:157:GLU:HA	1:F:160:TYR:CE2	2.46	0.51
1:H:194:ARG:HH21	1:H:209:THR:CB	2.24	0.51
1:E:138:MET:HE1	1:E:152:LEU:HD13	1.93	0.51
1:F:210:LEU:HG	1:F:227:LEU:HD21	1.93	0.50
1:H:156:LYS:NZ	1:H:176:ALA:O	2.44	0.50
1:D:109:ARG:N	1:D:227:LEU:O	2.41	0.50
1:G:129:ILE:HG22	1:G:173:PHE:CG	2.47	0.50
1:H:77:ASP:C	1:H:79:GLY:N	2.65	0.50
1:A:105:ARG:HH21	1:D:43:ARG:NH1	2.10	0.50
1:C:129:ILE:HG21	1:C:153:PHE:HD1	1.76	0.49
1:D:151:ILE:HG12	1:D:221:VAL:HG21	1.94	0.49
1:H:49:ARG:O	1:H:53:ILE:HG13	2.11	0.49
1:E:143:PRO:HD2	1:E:146:LEU:HD12	1.93	0.49
1:B:12:PRO:HB2	1:B:15:VAL:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:PRO:HD2	1:C:31:LEU:HD12	1.94	0.49
1:G:218:ARG:C	1:G:220:LEU:H	2.15	0.49
1:D:177:HIS:HB3	1:D:194:ARG:HB2	1.93	0.49
1:H:169:ARG:NH1	1:H:198:ASP:O	2.45	0.49
1:C:41:ILE:HD12	1:C:49:ARG:HG2	1.95	0.49
1:H:55:VAL:HG22	1:H:91:LEU:HD22	1.93	0.48
1:C:56:ARG:NH1	1:C:73:ILE:O	2.45	0.48
1:H:104:ARG:O	1:H:108:VAL:HG22	2.13	0.48
1:F:114:ASP:OD1	1:F:115:ALA:N	2.46	0.48
1:D:191:PHE:CZ	1:D:212:GLY:HA3	2.48	0.48
1:G:83:TRP:HH2	1:G:91:LEU:HD21	1.78	0.48
1:I:51:GLU:HG3	1:I:98:ARG:HH21	1.78	0.48
1:B:16:PHE:CD1	1:B:19:LEU:O	2.67	0.48
1:C:48:ARG:HH22	2:C:301:D16:CD	2.27	0.48
1:G:55:VAL:HG13	1:G:91:LEU:HD22	1.96	0.48
1:G:116:GLU:HB3	1:G:150:ARG:HD2	1.96	0.48
1:I:85:ASP:O	1:I:87:MET:HG2	2.13	0.48
1:A:143:PRO:HD2	1:A:146:LEU:HD12	1.96	0.47
1:I:181:GLU:OE1	1:I:190:ARG:NH2	2.48	0.47
1:C:132:PRO:HA	1:C:135:ARG:NH1	2.29	0.47
1:D:163:TRP:CE2	1:D:167:THR:HG21	2.50	0.47
1:H:7:VAL:HG13	1:H:97:TYR:OH	2.15	0.47
1:F:195:ILE:HD11	1:F:210:LEU:HD13	1.96	0.47
1:C:19:LEU:HD13	1:C:108:VAL:HG21	1.97	0.47
1:C:129:ILE:HA	1:C:173:PHE:HB3	1.97	0.46
1:I:129:ILE:HA	1:I:173:PHE:HB3	1.97	0.46
1:H:44:SER:HB3	1:H:48:ARG:HG2	1.97	0.46
1:I:129:ILE:HG13	1:I:130:SER:HB3	1.97	0.46
1:A:140:ARG:HD2	1:E:187:TRP:CD2	2.50	0.46
1:G:117:PRO:O	1:G:150:ARG:NH1	2.48	0.46
1:H:129:ILE:O	1:H:156:LYS:HE3	2.16	0.46
1:I:195:ILE:HD11	1:I:210:LEU:HD12	1.98	0.46
1:E:122:PRO:HD2	1:E:125:VAL:HG21	1.98	0.46
1:H:194:ARG:HH21	1:H:209:THR:HB	1.81	0.46
1:C:129:ILE:HG21	1:C:153:PHE:CD1	2.51	0.46
1:I:198:ASP:OD1	1:I:199:GLY:N	2.49	0.46
1:H:209:THR:O	1:H:210:LEU:HD22	2.16	0.45
1:F:114:ASP:OD2	1:F:154:CYS:HA	2.15	0.45
1:G:60:ARG:HA	1:G:63:LEU:HB2	1.97	0.45
1:G:169:ARG:HH22	1:G:200:SER:CB	2.13	0.45
1:B:129:ILE:O	1:B:156:LYS:HE3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:GLU:HB3	1:B:150:ARG:HD2	1.98	0.45
1:H:122:PRO:O	1:H:125:VAL:HG22	2.16	0.45
1:A:110:SER:HB3	1:A:227:LEU:HD12	1.96	0.45
1:I:71:ALA:HB3	1:I:84:PRO:HG3	1.98	0.45
1:G:193:SER:HB2	1:G:210:LEU:HB2	1.98	0.45
1:C:195:ILE:HB	1:C:208:THR:HG22	1.98	0.45
1:G:121:LEU:HD23	1:G:150:ARG:HE	1.82	0.45
1:H:77:ASP:O	1:H:79:GLY:N	2.43	0.45
1:A:67:GLY:HA3	1:B:190:ARG:NH1	2.33	0.44
1:B:121:LEU:HD12	1:B:149:ASP:HB2	1.99	0.44
1:A:55:VAL:HG22	1:A:91:LEU:HD22	2.00	0.44
1:G:83:TRP:CH2	1:G:91:LEU:HD21	2.52	0.44
1:C:143:PRO:HD2	1:C:146:LEU:HD12	1.99	0.44
1:G:218:ARG:O	1:G:220:LEU:N	2.50	0.44
1:D:163:TRP:HD1	1:D:207:LEU:HD23	1.82	0.44
1:I:159:THR:HG23	1:I:210:LEU:HD13	1.98	0.44
1:G:84:PRO:O	1:G:87:MET:HB2	2.18	0.44
1:G:187:TRP:HE3	1:G:216:VAL:HG21	1.82	0.44
1:A:28:PRO:HB2	1:A:31:LEU:HD23	1.99	0.44
1:D:36:GLU:OE1	1:D:36:GLU:N	2.46	0.44
1:D:207:LEU:HD21	1:D:210:LEU:HD11	2.00	0.44
1:H:177:HIS:N	1:H:194:ARG:O	2.51	0.43
1:E:48:ARG:HH22	2:E:301:D16:CD	2.31	0.43
1:E:116:GLU:HB3	1:E:150:ARG:HD2	2.00	0.43
1:E:135:ARG:HG3	1:E:148:TRP:CH2	2.52	0.43
1:A:6:LEU:HD21	1:A:218:ARG:HD3	2.00	0.43
1:E:26:SER:O	1:E:28:PRO:HD3	2.16	0.43
1:H:151:ILE:HG12	1:H:221:VAL:HG21	1.99	0.43
1:H:80:GLU:OE1	1:H:168:LYS:NZ	2.38	0.43
1:F:189:GLY:HA3	1:F:214:TRP:CE2	2.54	0.43
1:H:91:LEU:O	1:H:161:LYS:NZ	2.47	0.43
1:C:163:TRP:CE3	1:C:171:LEU:HB2	2.54	0.43
1:D:129:ILE:HA	1:D:173:PHE:CB	2.49	0.43
1:G:163:TRP:CE2	1:G:167:THR:HG21	2.54	0.43
1:H:110:SER:HB2	1:H:166:LEU:HD13	2.01	0.43
1:I:178:ILE:HA	1:I:192:VAL:O	2.19	0.43
1:H:195:ILE:HB	1:H:208:THR:HA	1.99	0.42
1:G:107:ALA:O	1:G:229:GLY:N	2.36	0.42
1:I:27:ASP:CG	1:I:50:ASN:HB3	2.39	0.42
1:H:191:PHE:CZ	1:H:212:GLY:HA3	2.54	0.42
1:A:20:ALA:HB2	1:A:66:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:ARG:HH11	1:D:43:ARG:HD2	1.66	0.42
1:D:63:LEU:HB3	1:D:68:VAL:HB	2.00	0.42
1:I:109:ARG:NH2	1:I:205:PRO:O	2.41	0.42
1:A:129:ILE:HA	1:A:173:PHE:HB3	2.02	0.42
1:G:27:ASP:CG	1:G:50:ASN:HB3	2.40	0.42
1:H:138:MET:SD	1:H:148:TRP:HB2	2.60	0.42
1:C:15:VAL:HG12	1:C:15:VAL:O	2.20	0.42
1:B:157:GLU:HA	1:B:160:TYR:CD2	2.55	0.42
1:C:121:LEU:HD12	1:C:149:ASP:HB2	2.02	0.42
1:I:97:TYR:CZ	1:I:222:LEU:HD11	2.53	0.42
1:B:163:TRP:CE3	1:B:171:LEU:HB2	2.55	0.41
1:E:105:ARG:HA	1:E:108:VAL:O	2.19	0.41
1:G:126:LEU:HD21	1:G:148:TRP:CH2	2.55	0.41
1:G:129:ILE:HG22	1:G:173:PHE:HB3	2.02	0.41
1:D:33:PRO:HG3	1:D:41:ILE:HD11	2.01	0.41
1:D:121:LEU:HD11	1:D:153:PHE:HB2	2.02	0.41
1:A:156:LYS:NZ	1:A:173:PHE:O	2.49	0.41
1:C:60:ARG:HD2	1:C:70:PRO:HB3	2.03	0.41
1:H:31:LEU:HB3	1:H:53:ILE:HG22	2.01	0.41
1:A:20:ALA:CB	1:A:65:GLN:HE21	2.31	0.41
1:H:61:ILE:O	1:H:65:GLN:HG2	2.20	0.41
1:E:28:PRO:HD2	1:E:31:LEU:HD12	2.03	0.41
1:G:187:TRP:HB3	1:G:216:VAL:CG2	2.48	0.41
1:H:121:LEU:HD13	1:H:125:VAL:HG23	2.02	0.41
1:A:28:PRO:O	1:A:31:LEU:HD23	2.20	0.41
1:A:27:ASP:CG	1:A:50:ASN:HB3	2.40	0.41
1:H:38:ALA:N	1:H:39:PRO:HD2	2.35	0.41
1:C:56:ARG:NH2	2:C:301:D16:CD	2.84	0.41
1:E:109:ARG:N	1:E:227:LEU:O	2.53	0.41
1:I:163:TRP:CE2	1:I:167:THR:HG21	2.56	0.41
1:B:137:ASP:OD1	1:C:187:TRP:HH2	2.05	0.40
1:E:43:ARG:NE	1:G:105:ARG:HH22	2.20	0.40
1:G:217:GLU:C	1:G:218:ARG:O	2.60	0.40
1:D:41:ILE:HB	1:D:49:ARG:HG2	2.02	0.40
1:D:163:TRP:CD1	1:D:207:LEU:HD23	2.56	0.40
1:E:41:ILE:O	1:E:49:ARG:NH1	2.54	0.40
1:H:129:ILE:HG21	1:H:153:PHE:CD1	2.53	0.40
1:I:83:TRP:HH2	1:I:91:LEU:HD21	1.86	0.40
1:I:138:MET:SD	1:I:152:LEU:HB2	2.61	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	216/235 (92%)	211 (98%)	5 (2%)	0	100	100
1	B	219/235 (93%)	214 (98%)	5 (2%)	0	100	100
1	C	223/235 (95%)	215 (96%)	8 (4%)	0	100	100
1	D	223/235 (95%)	213 (96%)	8 (4%)	2 (1%)	17	19
1	E	218/235 (93%)	217 (100%)	1 (0%)	0	100	100
1	F	81/235 (34%)	81 (100%)	0	0	100	100
1	G	189/235 (80%)	172 (91%)	14 (7%)	3 (2%)	9	8
1	H	208/235 (88%)	195 (94%)	11 (5%)	2 (1%)	15	16
1	I	209/235 (89%)	194 (93%)	14 (7%)	1 (0%)	29	34
All	All	1786/2115 (84%)	1712 (96%)	66 (4%)	8 (0%)	34	41

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	42	ALA
1	G	218	ARG
1	G	219	GLY
1	G	45	VAL
1	H	83	TRP
1	H	197	ILE
1	D	15	VAL
1	I	86	GLY

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	177/190 (93%)	174 (98%)	3 (2%)	60	73
1	B	179/190 (94%)	176 (98%)	3 (2%)	60	73
1	C	179/190 (94%)	175 (98%)	4 (2%)	52	64
1	D	163/190 (86%)	161 (99%)	2 (1%)	71	81
1	E	172/190 (90%)	168 (98%)	4 (2%)	50	63
1	F	65/190 (34%)	65 (100%)	0	100	100
1	G	156/190 (82%)	155 (99%)	1 (1%)	86	91
1	H	163/190 (86%)	160 (98%)	3 (2%)	59	71
1	I	171/190 (90%)	168 (98%)	3 (2%)	59	71
All	All	1425/1710 (83%)	1402 (98%)	23 (2%)	62	74

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ARG
1	A	160	TYR
1	A	190	ARG
1	B	135	ARG
1	B	160	TYR
1	B	213	ARG
1	C	56	ARG
1	C	160	TYR
1	C	190	ARG
1	C	203	SER
1	D	15	VAL
1	D	43	ARG
1	E	65	GLN
1	E	130	SER
1	E	160	TYR
1	E	194	ARG
1	G	48	ARG
1	H	78	LYS
1	H	85	ASP
1	H	109	ARG
1	I	56	ARG
1	I	190	ARG
1	I	213	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	123	ASN
1	E	65	GLN

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)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	D16	F	301	-	30,34,34	0.76	0	37,48,48	1.09	4 (10%)
2	D16	B	301	-	30,34,34	0.76	0	37,48,48	1.09	2 (5%)
2	D16	H	301	-	30,34,34	0.77	0	37,48,48	1.07	2 (5%)
2	D16	C	301	-	30,34,34	0.77	0	37,48,48	1.05	3 (8%)
2	D16	E	301	-	30,34,34	0.77	0	37,48,48	1.07	2 (5%)
2	D16	G	301	-	30,34,34	0.78	0	37,48,48	1.12	2 (5%)
2	D16	I	301	-	30,34,34	0.75	0	37,48,48	1.05	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	D16	A	301	-	30,34,34	0.74	0	37,48,48	1.05	3 (8%)
2	D16	D	301	-	30,34,34	0.76	0	37,48,48	1.08	3 (8%)

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	D16	F	301	-	-	4/19/25/25	0/3/3/3
2	D16	B	301	-	-	4/19/25/25	0/3/3/3
2	D16	H	301	-	-	3/19/25/25	0/3/3/3
2	D16	C	301	-	-	4/19/25/25	0/3/3/3
2	D16	E	301	-	-	3/19/25/25	0/3/3/3
2	D16	G	301	-	-	5/19/25/25	0/3/3/3
2	D16	I	301	-	-	4/19/25/25	0/3/3/3
2	D16	A	301	-	-	4/19/25/25	0/3/3/3
2	D16	D	301	-	-	2/19/25/25	0/3/3/3

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	D16	C8A-C4A-C4	-3.14	116.81	120.39
2	I	301	D16	C8A-C4A-C4	-3.14	116.81	120.39
2	F	301	D16	C8A-C4A-C4	-3.13	116.82	120.39
2	H	301	D16	C8A-C4A-C4	-3.11	116.85	120.39
2	A	301	D16	C8A-C4A-C4	-3.10	116.85	120.39
2	E	301	D16	C8A-C4A-C4	-3.07	116.89	120.39
2	G	301	D16	C8A-C4A-C4	-3.07	116.89	120.39
2	C	301	D16	C8A-C4A-C4	-2.96	117.01	120.39
2	D	301	D16	C8A-C4A-C4	-2.94	117.04	120.39
2	I	301	D16	O4-C4-N3	-2.72	117.37	120.59
2	A	301	D16	O4-C4-N3	-2.63	117.47	120.59
2	F	301	D16	O4-C4-N3	-2.63	117.47	120.59
2	B	301	D16	O4-C4-N3	-2.62	117.48	120.59
2	E	301	D16	O4-C4-N3	-2.60	117.50	120.59
2	G	301	D16	O4-C4-N3	-2.52	117.60	120.59
2	H	301	D16	O4-C4-N3	-2.46	117.67	120.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	D16	O4-C4-N3	-2.39	117.75	120.59
2	D	301	D16	O4-C4-N3	-2.28	117.88	120.59
2	D	301	D16	C6-C9-N10	-2.21	111.07	113.81
2	C	301	D16	C4A-C8A-N1	-2.10	117.85	119.49
2	F	301	D16	C4A-C8A-N1	-2.09	117.85	119.49
2	F	301	D16	C4A-C4-N3	2.03	120.74	117.88
2	A	301	D16	C4A-C8A-N1	-2.01	117.92	119.49

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	301	D16	CB-CA-CT-O1
2	G	301	D16	CB-CA-CT-O2
2	H	301	D16	CT-CA-CB-CG
2	C	301	D16	CB-CA-CT-O2
2	C	301	D16	CB-CA-CT-O1
2	I	301	D16	CB-CA-CT-O2
2	B	301	D16	CB-CA-CT-O1
2	B	301	D16	CB-CA-CT-O2
2	E	301	D16	CT-CA-CB-CG
2	G	301	D16	CT-CA-CB-CG
2	I	301	D16	CB-CA-CT-O1
2	H	301	D16	OE2-CD-CG-CB
2	C	301	D16	OE2-CD-CG-CB
2	E	301	D16	OE1-CD-CG-CB
2	H	301	D16	OE1-CD-CG-CB
2	D	301	D16	OE1-CD-CG-CB
2	E	301	D16	OE2-CD-CG-CB
2	G	301	D16	OE2-CD-CG-CB
2	I	301	D16	OE1-CD-CG-CB
2	I	301	D16	OE2-CD-CG-CB
2	C	301	D16	OE1-CD-CG-CB
2	G	301	D16	OE1-CD-CG-CB
2	A	301	D16	CB-CA-CT-O2
2	D	301	D16	OE2-CD-CG-CB
2	F	301	D16	OE2-CD-CG-CB
2	F	301	D16	OE1-CD-CG-CB
2	F	301	D16	CB-CA-CT-O1
2	A	301	D16	OE2-CD-CG-CB
2	B	301	D16	OE2-CD-CG-CB
2	A	301	D16	OE1-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
2	B	301	D16	OE1-CD-CG-CB
2	A	301	D16	CB-CA-CT-O1
2	F	301	D16	CB-CA-CT-O2

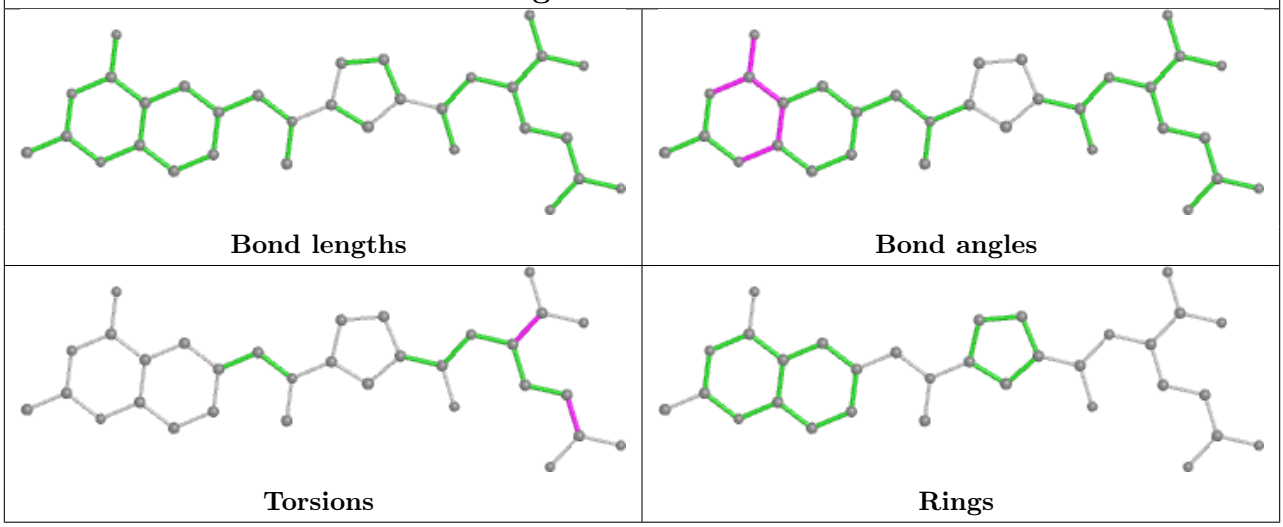
There are no ring outliers.

4 monomers are involved in 8 short contacts:

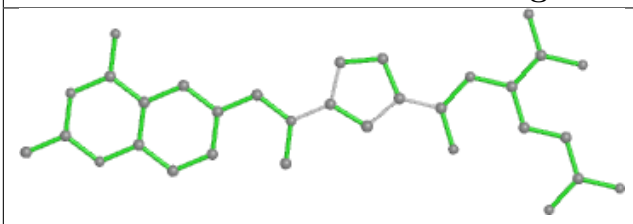
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	301	D16	2	0
2	C	301	D16	2	0
2	E	301	D16	2	0
2	G	301	D16	2	0

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 D16 F 301



Ligand D16 B 301



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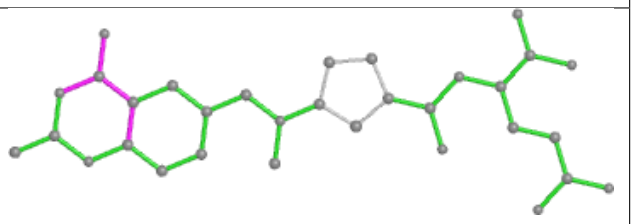
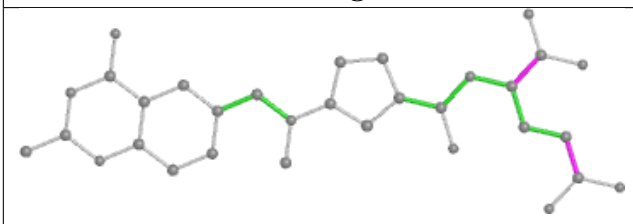
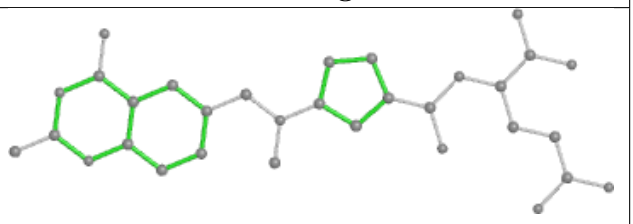


Bond angles

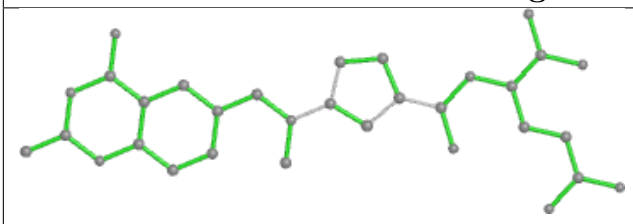


Torsions



Rings

Ligand D16 H 301



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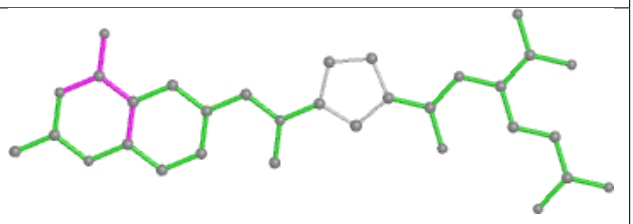
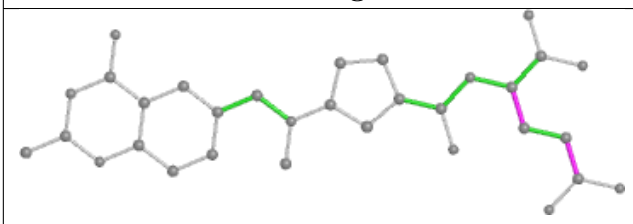


Bond angles



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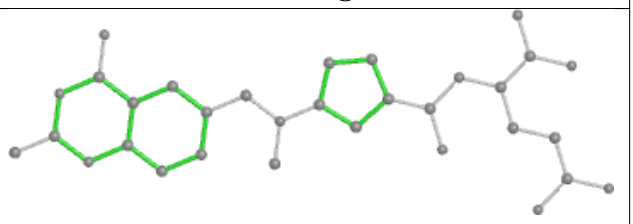
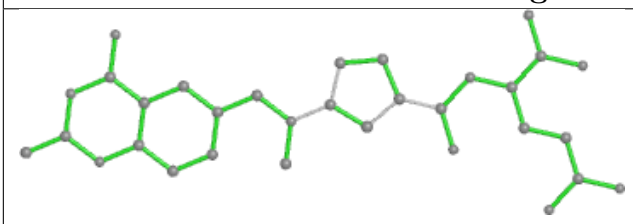
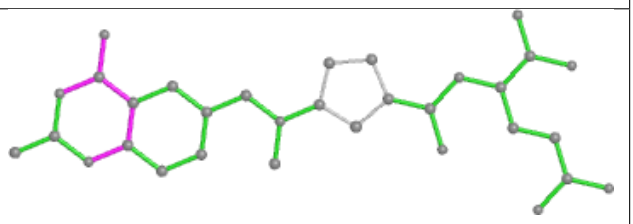


Rings

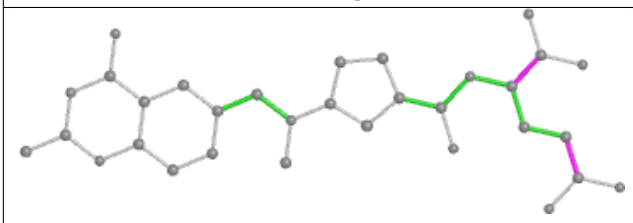
Ligand D16 C 301



Bond lengths



Bond angles



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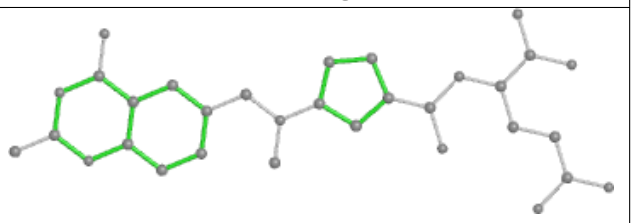
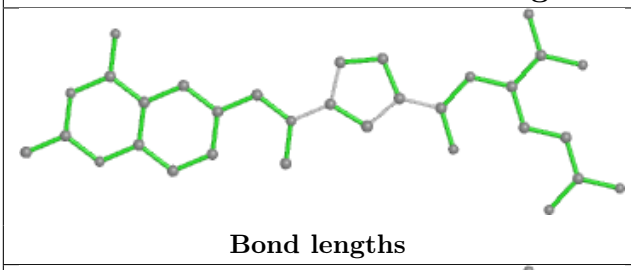
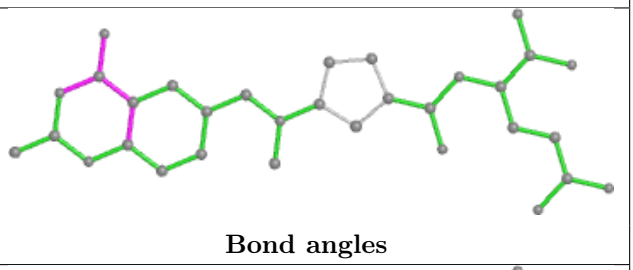


Rings

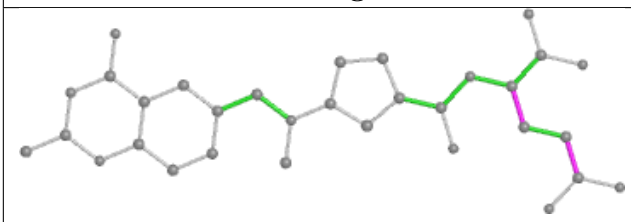
Ligand D16 E 301



Bond lengths



Bond angles



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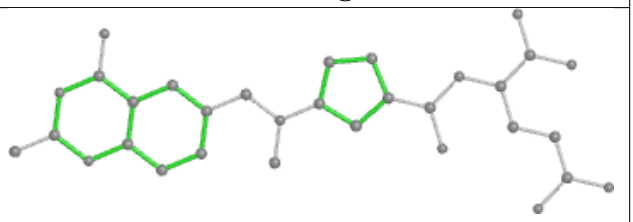
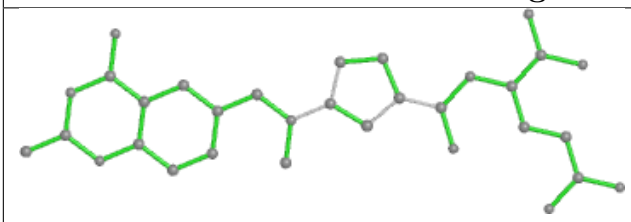
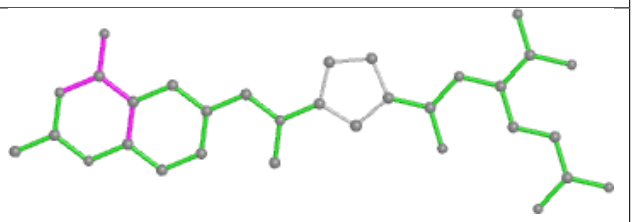


Rings

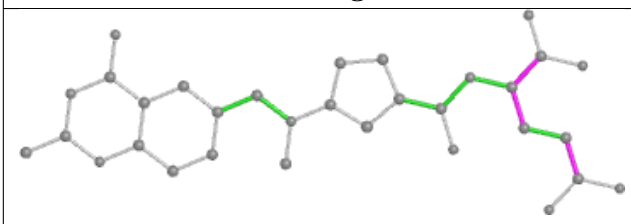
Ligand D16 G 301



Bond lengths



Bond angles



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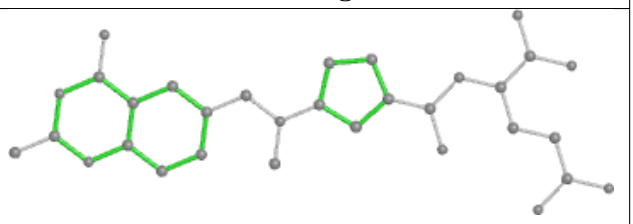
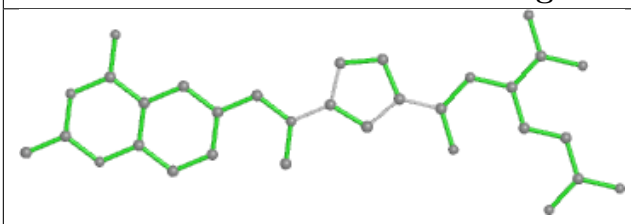


Rings

Ligand D16 I 301



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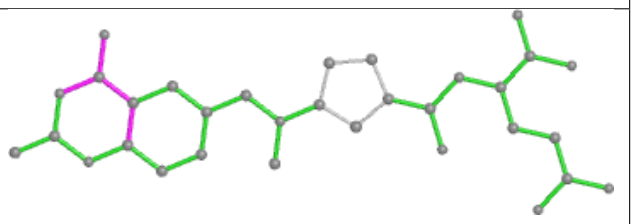
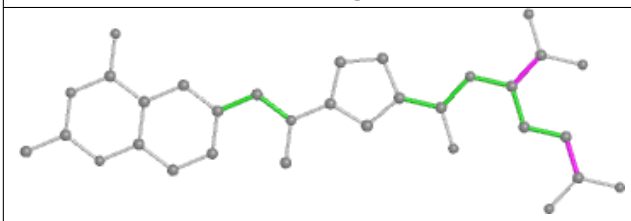


Bond angles



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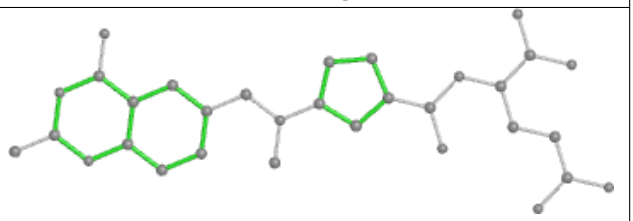
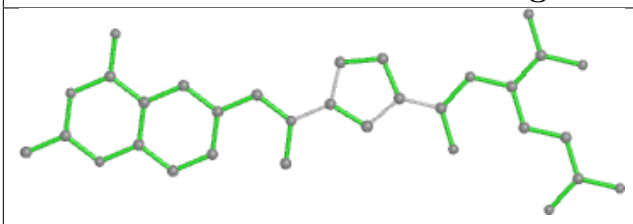


Rings

Ligand D16 A 301



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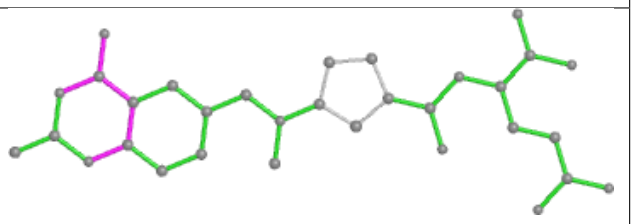
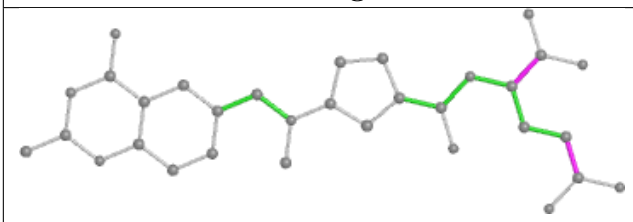


Bond angles



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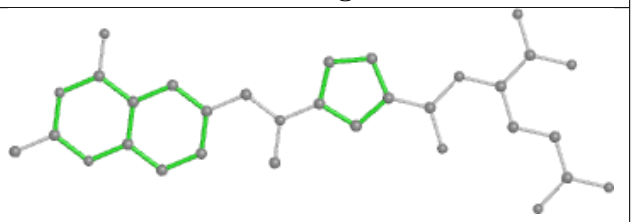
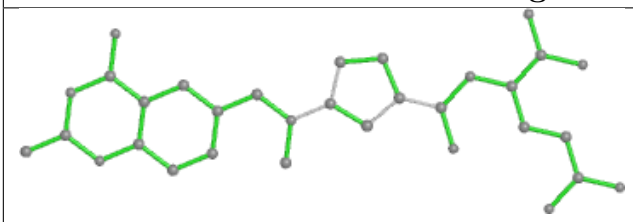
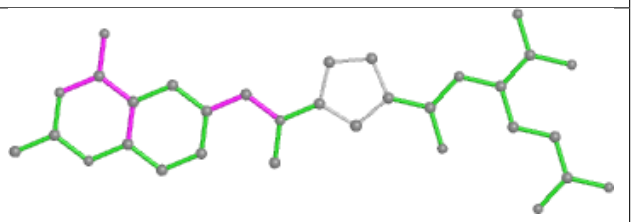


Rings

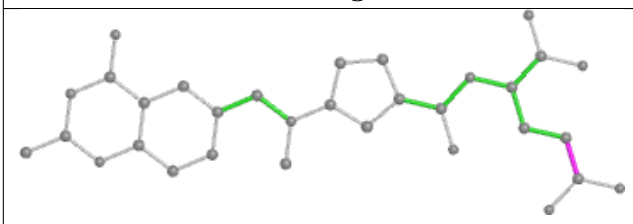
Ligand D16 D 301



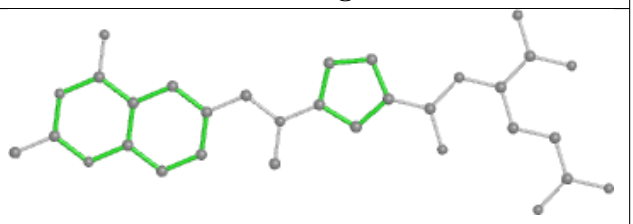
Bond lengths



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	220/235 (93%)	0.28	7 (3%) 47 44	25, 40, 55, 71	0
1	B	223/235 (94%)	0.23	11 (4%) 29 27	21, 37, 54, 73	0
1	C	225/235 (95%)	0.51	13 (5%) 23 20	21, 43, 67, 88	0
1	D	225/235 (95%)	0.63	20 (8%) 9 6	25, 46, 75, 83	0
1	E	222/235 (94%)	0.35	9 (4%) 37 34	24, 42, 60, 69	0
1	F	97/235 (41%)	1.68	34 (35%) 0 0	42, 60, 71, 78	0
1	G	197/235 (83%)	0.90	30 (15%) 2 1	35, 53, 69, 80	0
1	H	216/235 (91%)	0.83	25 (11%) 4 3	34, 51, 74, 82	0
1	I	217/235 (92%)	0.88	29 (13%) 3 2	33, 51, 74, 82	0
All	All	1842/2115 (87%)	0.63	178 (9%) 7 5	21, 46, 71, 88	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	69	PRO	5.8
1	G	122	PRO	5.5
1	B	16	PHE	5.3
1	F	175	ASP	5.1
1	E	14	THR	5.0
1	I	53	ILE	4.8
1	C	144	ALA	4.7
1	I	204	GLY	4.6
1	H	35	PRO	4.6
1	I	203	SER	4.6
1	H	18	ASP	4.5
1	F	110	SER	4.3
1	G	128	ALA	4.3
1	F	185	THR	4.2
1	I	68	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	148	TRP	4.1
1	H	29	PRO	4.0
1	H	69	PRO	4.0
1	F	207	LEU	4.0
1	A	123	ASN	3.9
1	D	13	ALA	3.9
1	G	185	THR	3.9
1	H	46	ALA	3.9
1	I	69	PRO	3.8
1	F	123	ASN	3.8
1	G	69	PRO	3.7
1	F	178	ILE	3.7
1	C	14	THR	3.6
1	C	13	ALA	3.6
1	I	106	ASP	3.6
1	H	206	PRO	3.6
1	C	140	ARG	3.5
1	E	29	PRO	3.5
1	I	39	PRO	3.4
1	H	82	CYS	3.4
1	F	120	VAL	3.4
1	G	148	TRP	3.4
1	F	170	TRP	3.3
1	B	15	VAL	3.3
1	F	227	LEU	3.2
1	F	220	LEU	3.2
1	F	184	SER	3.2
1	I	64	ASP	3.2
1	F	73	ILE	3.1
1	A	204	GLY	3.1
1	H	64	ASP	3.1
1	F	90	SER	3.1
1	H	60	ARG	3.1
1	D	16	PHE	3.1
1	E	185	THR	3.1
1	F	206	PRO	3.1
1	I	70	PRO	3.1
1	G	229	GLY	3.1
1	E	13	ALA	3.0
1	I	57	HIS	3.0
1	C	123	ASN	3.0
1	F	12	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	182	THR	3.0
1	C	122	PRO	3.0
1	D	135	ARG	3.0
1	D	17	GLU	3.0
1	D	138	MET	2.9
1	F	191	PHE	2.9
1	I	123	ASN	2.9
1	D	14	THR	2.9
1	H	17	GLU	2.9
1	C	132	PRO	2.9
1	F	121	LEU	2.9
1	G	120	VAL	2.9
1	B	203	SER	2.9
1	G	124	GLY	2.9
1	H	228	ALA	2.9
1	D	122	PRO	2.8
1	I	228	ALA	2.8
1	F	192	VAL	2.8
1	F	155	ALA	2.8
1	H	106	ASP	2.8
1	F	158	ALA	2.8
1	F	179	THR	2.8
1	I	26	SER	2.8
1	C	29	PRO	2.8
1	D	139	PRO	2.8
1	E	106	ASP	2.8
1	I	28	PRO	2.7
1	I	99	GLY	2.7
1	I	113	ILE	2.7
1	G	35	PRO	2.7
1	C	106	ASP	2.7
1	H	108	VAL	2.7
1	H	207	LEU	2.7
1	H	107	ALA	2.6
1	C	139	PRO	2.6
1	F	8	ALA	2.6
1	F	150	ARG	2.6
1	F	149	ASP	2.6
1	G	21	TYR	2.5
1	A	17	GLU	2.5
1	G	127	ASP	2.5
1	I	65	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	155	ALA	2.5
1	E	85	ASP	2.5
1	G	125	VAL	2.5
1	H	91	LEU	2.5
1	F	208	THR	2.5
1	C	67	GLY	2.5
1	D	123	ASN	2.5
1	D	211	ARG	2.5
1	G	184	SER	2.5
1	I	59	ALA	2.5
1	G	169	ARG	2.4
1	H	83	TRP	2.4
1	I	29	PRO	2.4
1	I	47	LYS	2.4
1	D	140	ARG	2.4
1	D	141	THR	2.4
1	G	177	HIS	2.4
1	B	127	ASP	2.4
1	F	6	LEU	2.4
1	F	118	HIS	2.3
1	H	84	PRO	2.3
1	E	133	ALA	2.3
1	I	185	THR	2.3
1	G	68	VAL	2.3
1	H	205	PRO	2.3
1	H	197	ILE	2.3
1	B	123	ASN	2.3
1	D	120	VAL	2.3
1	G	91	LEU	2.3
1	G	123	ASN	2.3
1	D	136	ALA	2.3
1	I	107	ALA	2.3
1	I	92	THR	2.3
1	A	70	PRO	2.3
1	F	112	GLY	2.3
1	F	209	THR	2.3
1	G	159	THR	2.3
1	H	70	PRO	2.2
1	H	122	PRO	2.2
1	A	101	VAL	2.2
1	G	106	ASP	2.2
1	D	124	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	71	ALA	2.2
1	G	105	ARG	2.2
1	F	224	ALA	2.2
1	B	229	GLY	2.2
1	B	17	GLU	2.2
1	G	224	ALA	2.1
1	A	113	ILE	2.1
1	G	112	GLY	2.1
1	A	218	ARG	2.1
1	I	56	ARG	2.1
1	G	95	ALA	2.1
1	H	73	ILE	2.1
1	D	145	ALA	2.1
1	D	228	ALA	2.1
1	G	162	ALA	2.1
1	H	65	GLN	2.1
1	G	18	ASP	2.1
1	D	185	THR	2.1
1	E	35	PRO	2.1
1	I	218	ARG	2.1
1	B	113	ILE	2.1
1	C	187	TRP	2.1
1	B	185	THR	2.1
1	H	178	ILE	2.1
1	I	74	LEU	2.1
1	I	112	GLY	2.1
1	G	194	ARG	2.1
1	E	46	ALA	2.0
1	F	74	LEU	2.0
1	C	69	PRO	2.0
1	I	100	ALA	2.0
1	D	15	VAL	2.0
1	F	223	THR	2.0
1	I	158	ALA	2.0
1	G	223	THR	2.0
1	F	7	VAL	2.0
1	B	204	GLY	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)

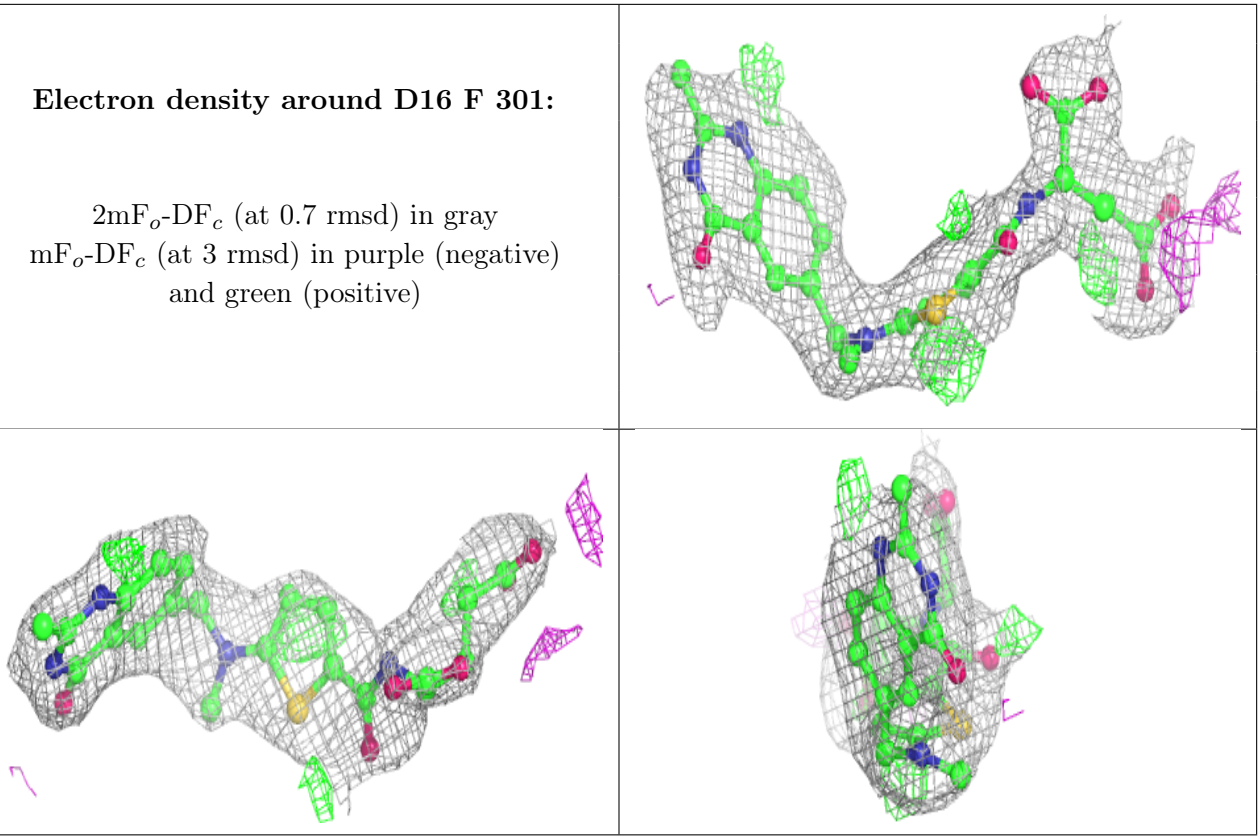
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	D16	F	301	32/32	0.87	0.19	36,48,58,61	0
2	D16	D	301	32/32	0.93	0.14	24,30,36,41	0
2	D16	G	301	32/32	0.93	0.15	33,38,46,47	0
2	D16	I	301	32/32	0.93	0.15	30,43,54,58	0
2	D16	E	301	32/32	0.95	0.14	25,30,39,40	0
2	D16	B	301	32/32	0.95	0.13	17,26,36,40	0
2	D16	C	301	32/32	0.95	0.14	22,27,32,38	0
2	D16	H	301	32/32	0.95	0.15	32,41,48,51	0
2	D16	A	301	32/32	0.95	0.13	19,28,33,38	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.

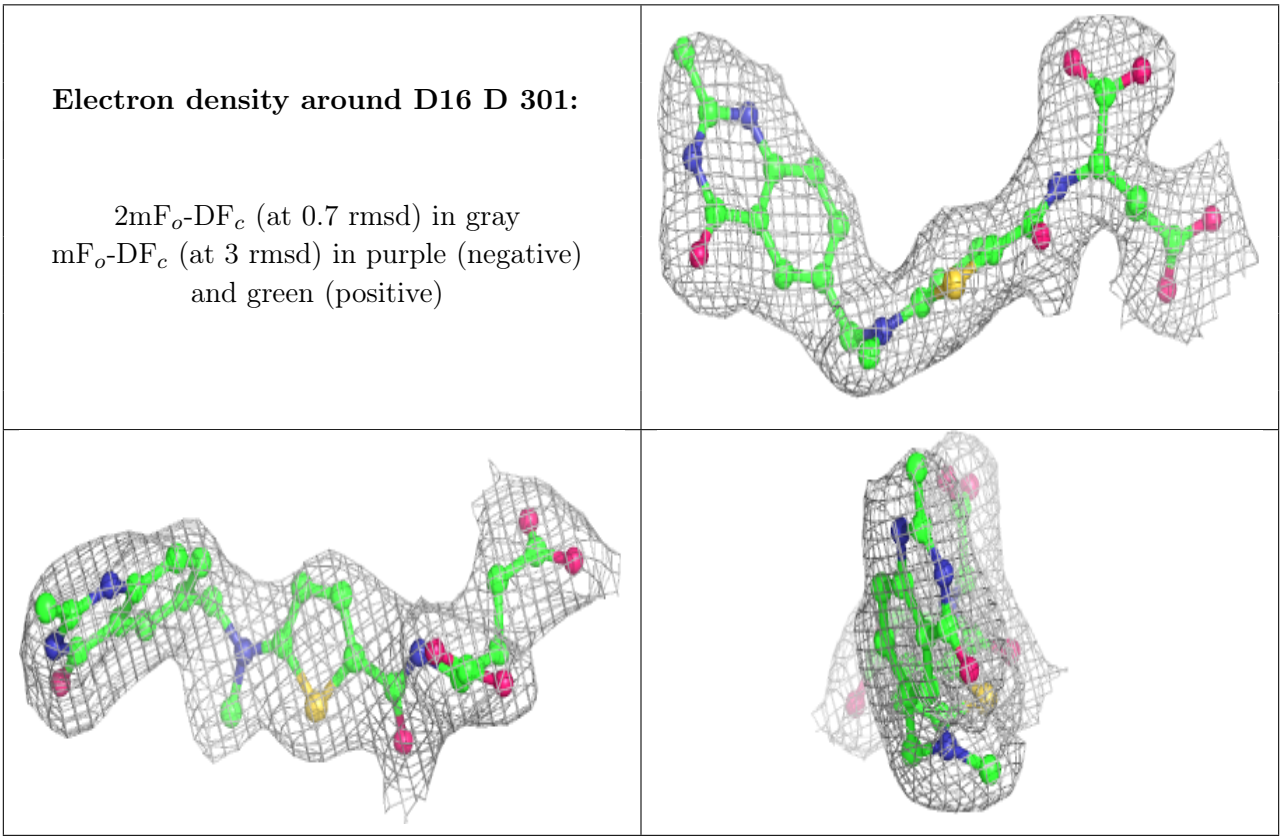
Electron density around D16 F 301:

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



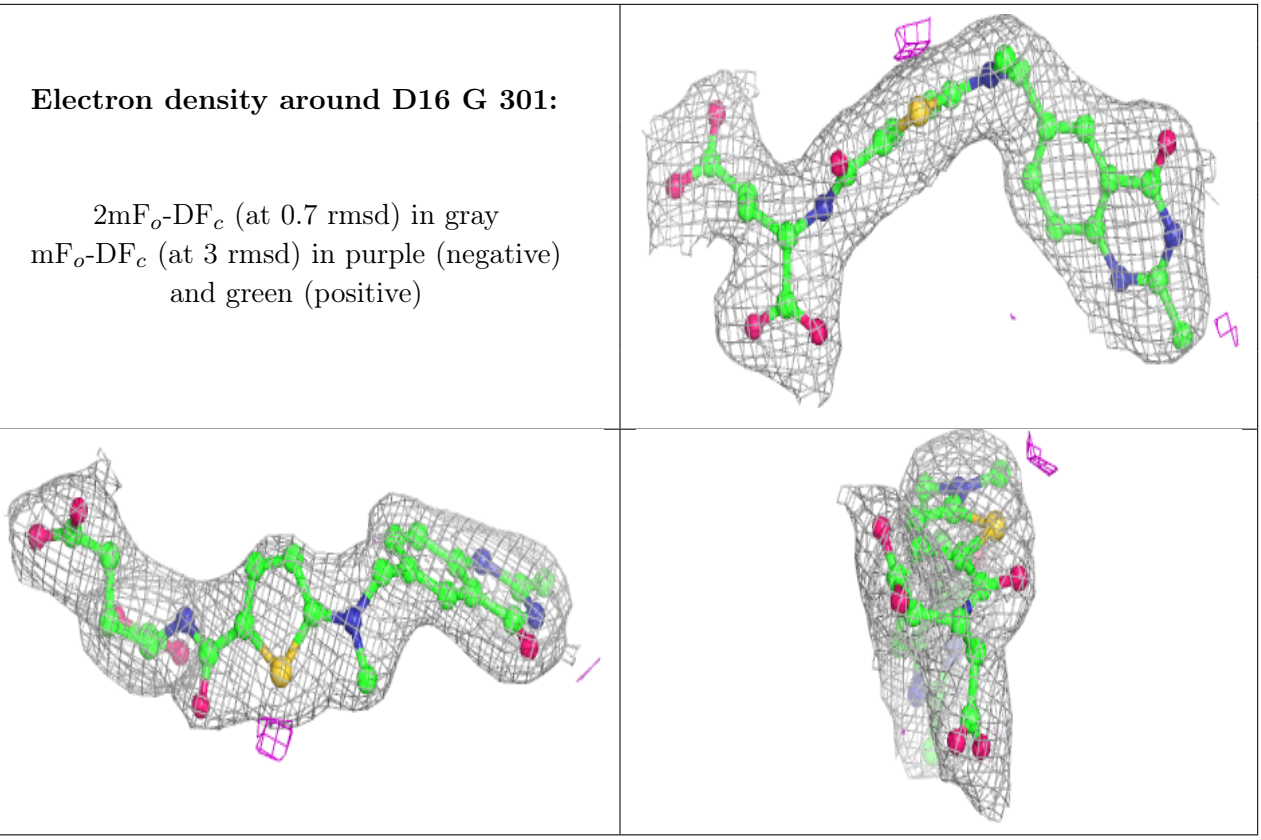
Electron density around D16 D 301:

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



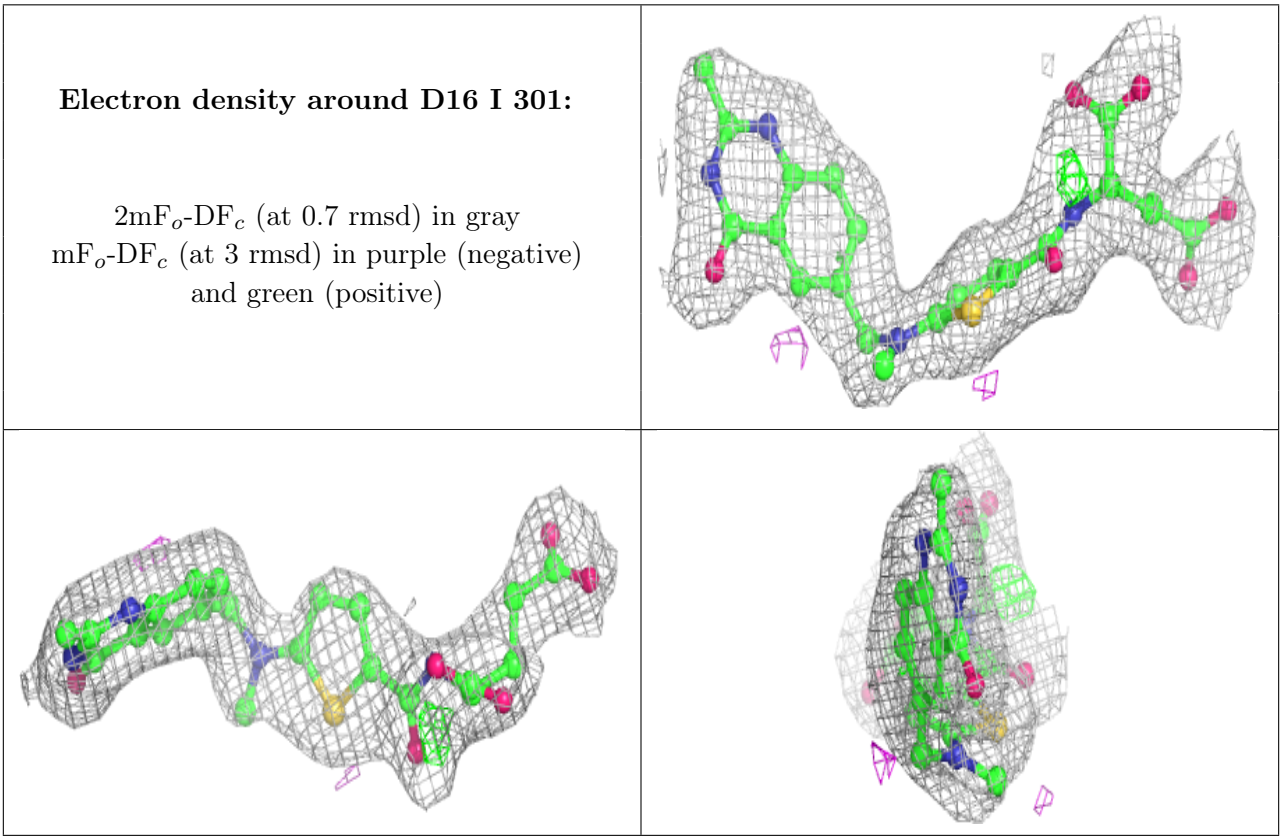
Electron density around D16 G 301:

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



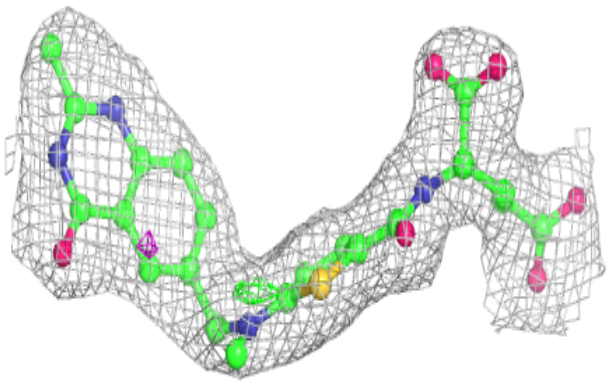
Electron density around D16 I 301:

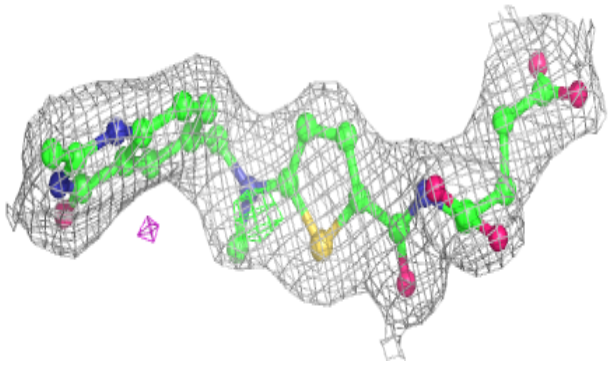
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

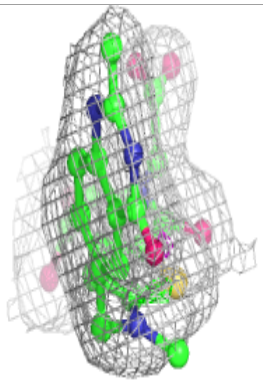


Electron density around D16 E 301:

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

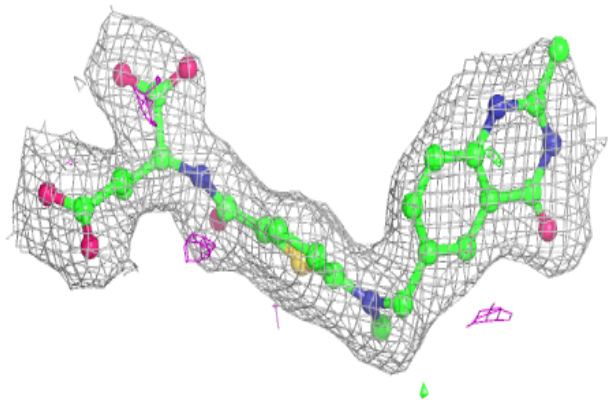


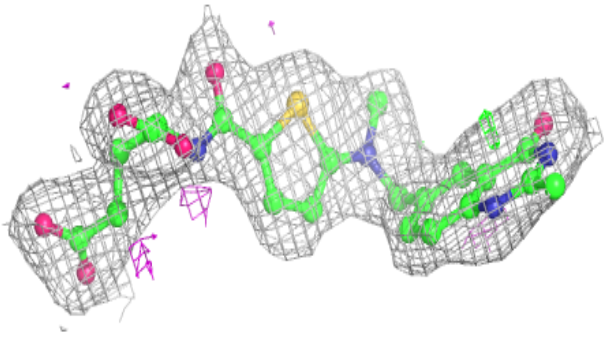


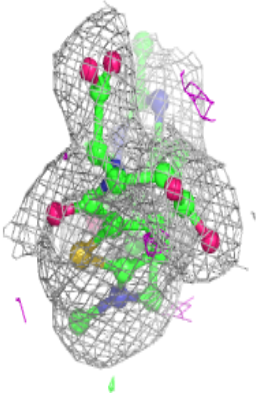


Electron density around D16 B 301:

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

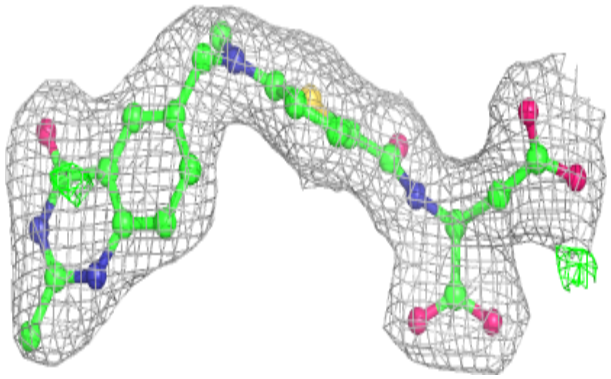


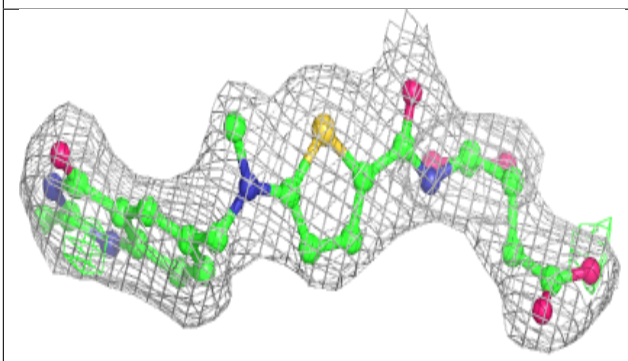


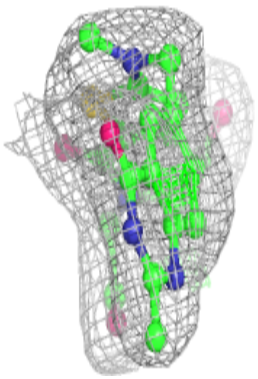


Electron density around D16 C 301:

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

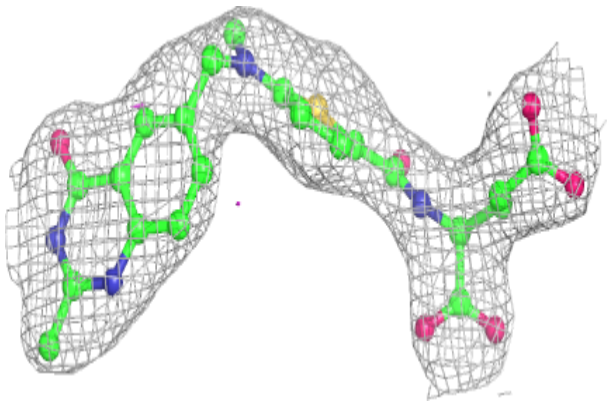


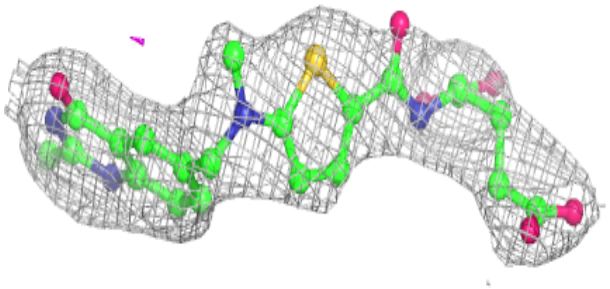


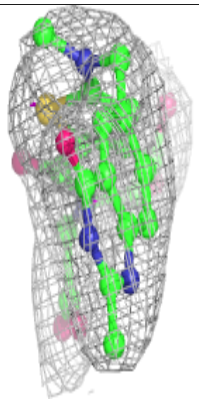


Electron density around D16 H 301:

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

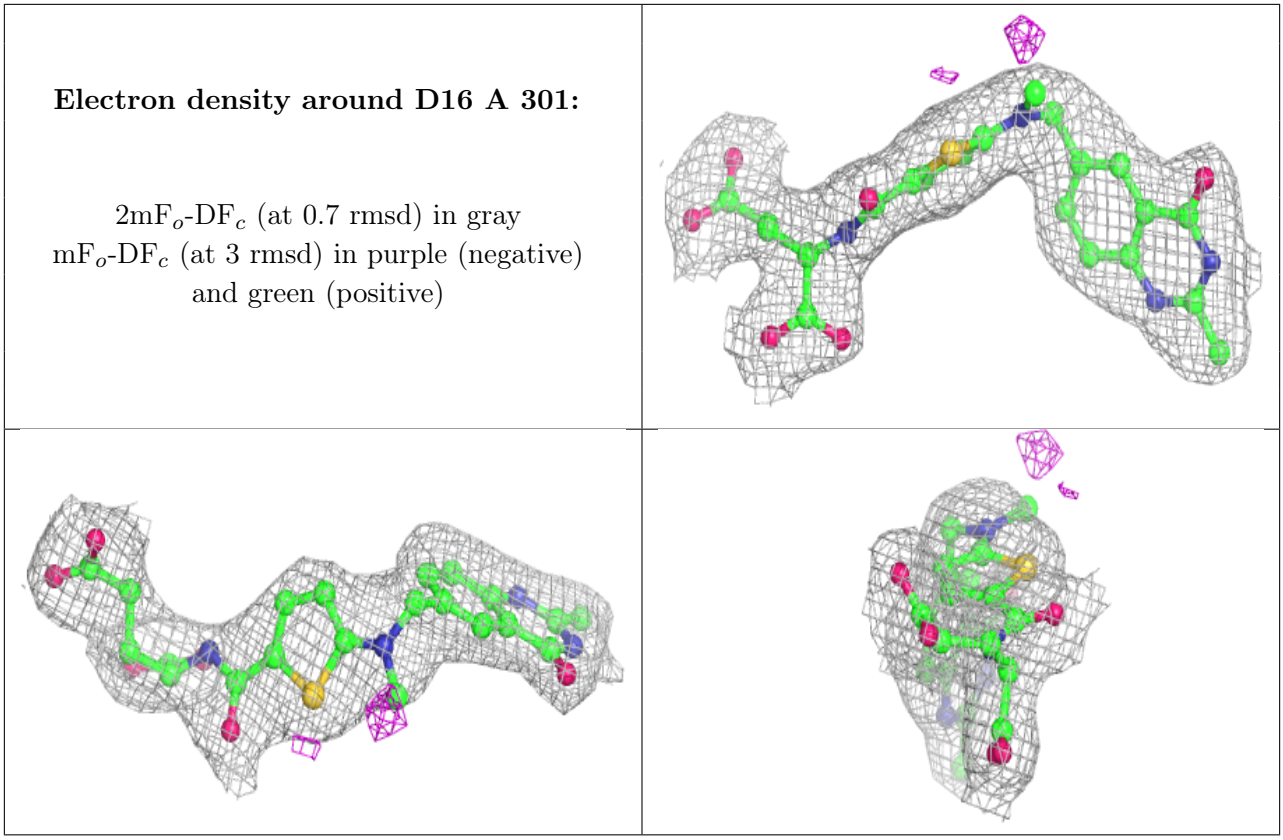






Electron density around D16 A 301:

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



6.5 Other polymers (i)

There are no such residues in this entry.