Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2026 – 03:33 pm GMT

PDB ID	:	30EJ / pdb_000030ej
Title	:	2-heptyl-4(1H)-quinolone synthase PqsBC in complex with compound 33
Authors	:	Borgert, S.R.; Blankenfeldt, W.
Deposited on	:	2026-04-21
Resolution	:	2.06 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 (i) 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 (i)) were used in the production of this report:

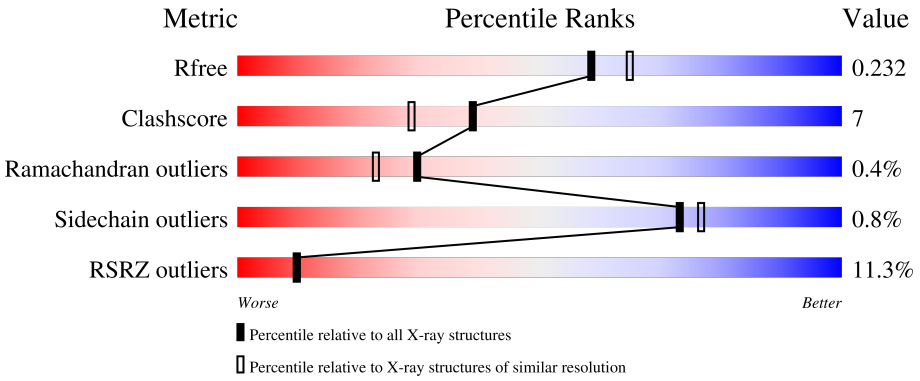
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.06 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.



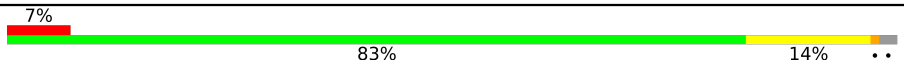
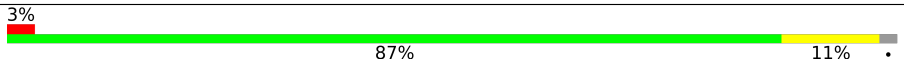
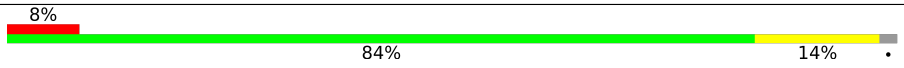
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	365	9% 82% 15% .
1	C	365	14% 75% 19% . .
1	E	365	8% 81% 14% . .
1	G	365	32% 73% 22% 5%
2	B	283	% 90% 9% .

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Mol	Chain	Length	Quality of chain
2	D	283	
2	F	283	
2	H	283	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 19912 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 2-heptyl-4(1H)-quinolone synthase subunit PqsC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	2	0
			2753	1743	478	513	19			
1	C	350	Total	C	N	O	S	0	1	0
			2701	1710	464	508	19			
1	E	349	Total	C	N	O	S	0	1	0
			2710	1719	468	504	19			
1	G	346	Total	C	N	O	S	0	0	0
			2657	1689	451	498	19			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP Q9I4X1
A	-15	GLY	-	expression tag	UNP Q9I4X1
A	-14	HIS	-	expression tag	UNP Q9I4X1
A	-13	HIS	-	expression tag	UNP Q9I4X1
A	-12	HIS	-	expression tag	UNP Q9I4X1
A	-11	HIS	-	expression tag	UNP Q9I4X1
A	-10	HIS	-	expression tag	UNP Q9I4X1
A	-9	HIS	-	expression tag	UNP Q9I4X1
A	-8	ALA	-	expression tag	UNP Q9I4X1
A	-7	GLU	-	expression tag	UNP Q9I4X1
A	-6	ASN	-	expression tag	UNP Q9I4X1
A	-5	LEU	-	expression tag	UNP Q9I4X1
A	-4	TYR	-	expression tag	UNP Q9I4X1
A	-3	PHE	-	expression tag	UNP Q9I4X1
A	-2	GLN	-	expression tag	UNP Q9I4X1
A	-1	GLY	-	expression tag	UNP Q9I4X1
A	0	HIS	-	expression tag	UNP Q9I4X1
C	-16	MET	-	initiating methionine	UNP Q9I4X1
C	-15	GLY	-	expression tag	UNP Q9I4X1
C	-14	HIS	-	expression tag	UNP Q9I4X1
C	-13	HIS	-	expression tag	UNP Q9I4X1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP Q9I4X1
C	-11	HIS	-	expression tag	UNP Q9I4X1
C	-10	HIS	-	expression tag	UNP Q9I4X1
C	-9	HIS	-	expression tag	UNP Q9I4X1
C	-8	ALA	-	expression tag	UNP Q9I4X1
C	-7	GLU	-	expression tag	UNP Q9I4X1
C	-6	ASN	-	expression tag	UNP Q9I4X1
C	-5	LEU	-	expression tag	UNP Q9I4X1
C	-4	TYR	-	expression tag	UNP Q9I4X1
C	-3	PHE	-	expression tag	UNP Q9I4X1
C	-2	GLN	-	expression tag	UNP Q9I4X1
C	-1	GLY	-	expression tag	UNP Q9I4X1
C	0	HIS	-	expression tag	UNP Q9I4X1
E	-16	MET	-	initiating methionine	UNP Q9I4X1
E	-15	GLY	-	expression tag	UNP Q9I4X1
E	-14	HIS	-	expression tag	UNP Q9I4X1
E	-13	HIS	-	expression tag	UNP Q9I4X1
E	-12	HIS	-	expression tag	UNP Q9I4X1
E	-11	HIS	-	expression tag	UNP Q9I4X1
E	-10	HIS	-	expression tag	UNP Q9I4X1
E	-9	HIS	-	expression tag	UNP Q9I4X1
E	-8	ALA	-	expression tag	UNP Q9I4X1
E	-7	GLU	-	expression tag	UNP Q9I4X1
E	-6	ASN	-	expression tag	UNP Q9I4X1
E	-5	LEU	-	expression tag	UNP Q9I4X1
E	-4	TYR	-	expression tag	UNP Q9I4X1
E	-3	PHE	-	expression tag	UNP Q9I4X1
E	-2	GLN	-	expression tag	UNP Q9I4X1
E	-1	GLY	-	expression tag	UNP Q9I4X1
E	0	HIS	-	expression tag	UNP Q9I4X1
G	-16	MET	-	initiating methionine	UNP Q9I4X1
G	-15	GLY	-	expression tag	UNP Q9I4X1
G	-14	HIS	-	expression tag	UNP Q9I4X1
G	-13	HIS	-	expression tag	UNP Q9I4X1
G	-12	HIS	-	expression tag	UNP Q9I4X1
G	-11	HIS	-	expression tag	UNP Q9I4X1
G	-10	HIS	-	expression tag	UNP Q9I4X1
G	-9	HIS	-	expression tag	UNP Q9I4X1
G	-8	ALA	-	expression tag	UNP Q9I4X1
G	-7	GLU	-	expression tag	UNP Q9I4X1
G	-6	ASN	-	expression tag	UNP Q9I4X1
G	-5	LEU	-	expression tag	UNP Q9I4X1

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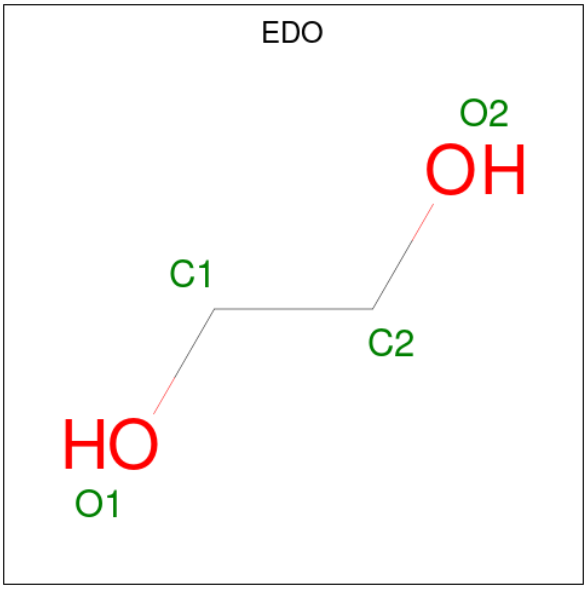
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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	TYR	-	expression tag	UNP Q9I4X1
G	-3	PHE	-	expression tag	UNP Q9I4X1
G	-2	GLN	-	expression tag	UNP Q9I4X1
G	-1	GLY	-	expression tag	UNP Q9I4X1
G	0	HIS	-	expression tag	UNP Q9I4X1

- Molecule 2 is a protein called 2-heptyl-4(1H)-quinolone synthase subunit PqsB.

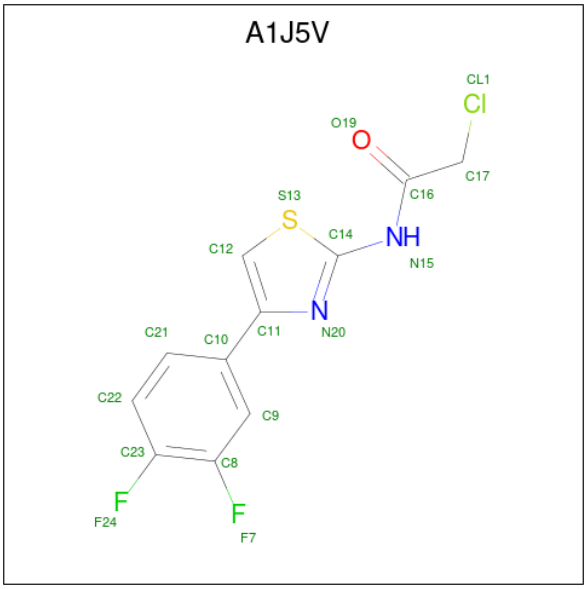
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	279	Total	C	N	O	S	0	0	0
			2117	1335	378	396	8			
2	D	278	Total	C	N	O	S	0	0	0
			2109	1331	376	394	8			
2	F	278	Total	C	N	O	S	0	2	0
			2133	1344	383	398	8			
2	H	278	Total	C	N	O	S	0	1	0
			2116	1335	376	397	8			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is N-[4-[3,4-bis(fluoranyl)phenyl]-1,3-thiazol-2-yl]-2-chloranyl-ethanamide (CCD ID: A1J5V) (formula: $C_{11}H_7ClF_2N_2OS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	S	0	0
			17	11	2	2	1	1		
4	C	1	Total	C	F	N	O	S	0	0
			17	11	2	2	1	1		
4	E	1	Total	C	F	N	O	S	0	0
			17	11	2	2	1	1		
4	G	1	Total	C	F	N	O	S	0	0
			17	11	2	2	1	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	123	Total	O	0	0
			123	123		
6	B	142	Total	O	0	0
			142	142		
6	C	18	Total	O	0	0
			18	18		

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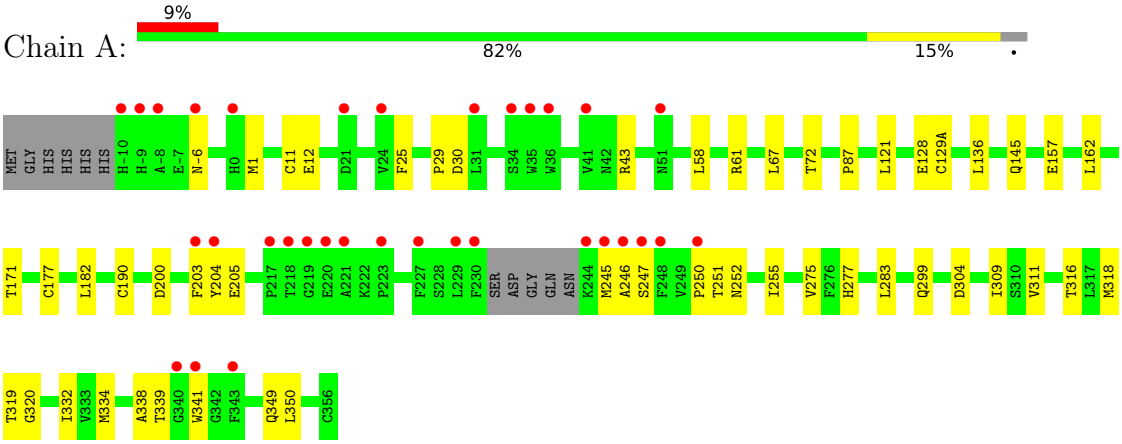
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	33	Total O 33 33	0	0
6	E	58	Total O 58 58	0	0
6	F	104	Total O 104 104	0	0
6	G	5	Total O 5 5	0	0
6	H	56	Total O 56 56	0	0

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.

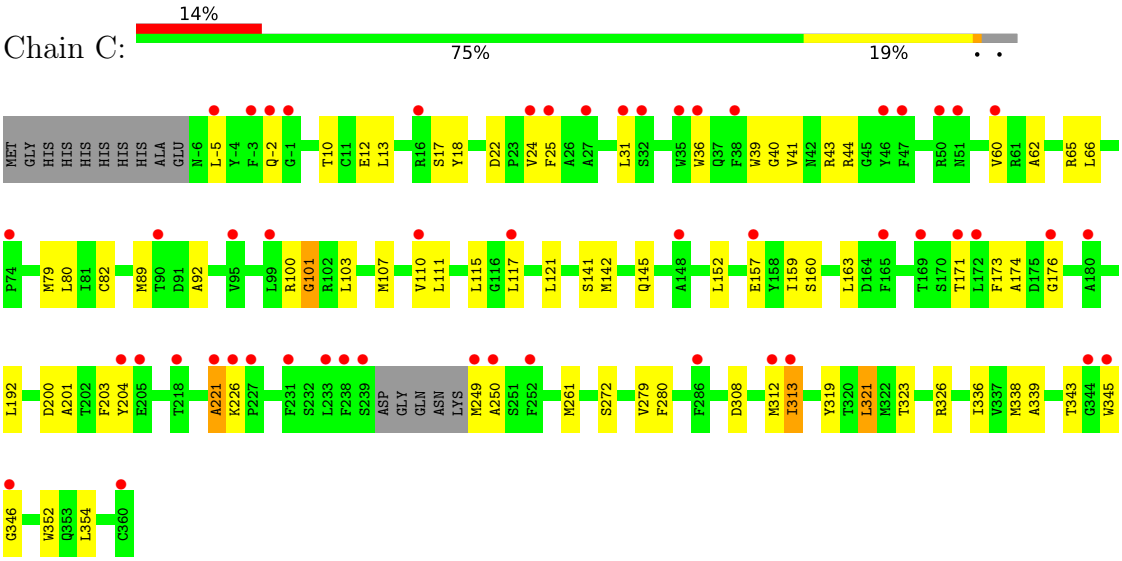
• Molecule 1: 2-heptyl-4(1H)-quinolone synthase subunit PqsC

Chain A:



• Molecule 1: 2-heptyl-4(1H)-quinolone synthase subunit PqsC

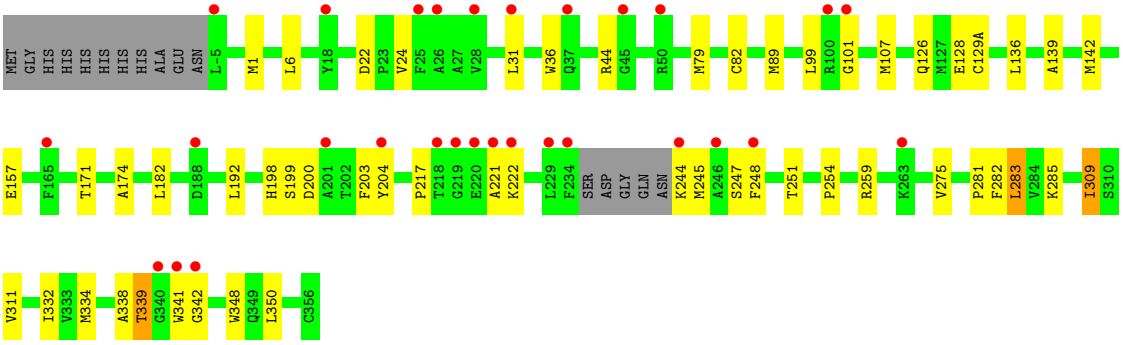
Chain C:



• Molecule 1: 2-heptyl-4(1H)-quinolone synthase subunit PqsC

Chain E:

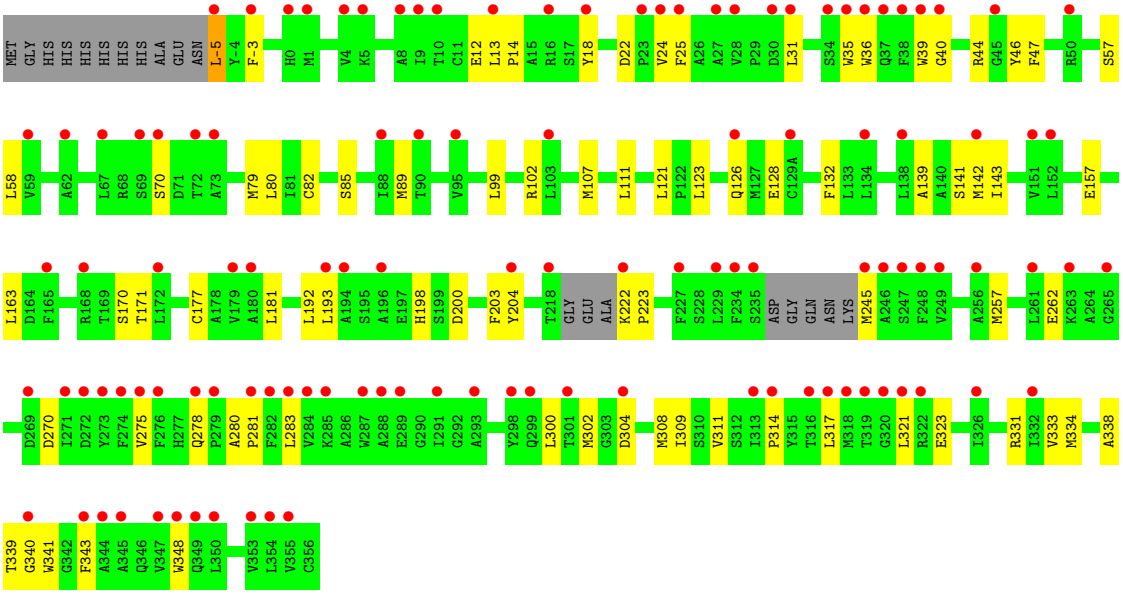




• Molecule 1: 2-heptyl-4(1H)-quinolone synthase subunit PqsC

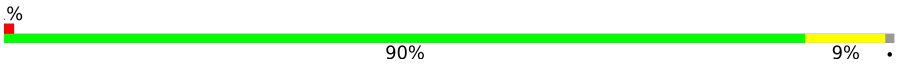
Chain G:

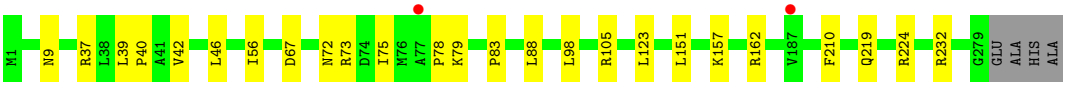




• Molecule 2: 2-heptyl-4(1H)-quinolone synthase subunit PqsB

Chain B:

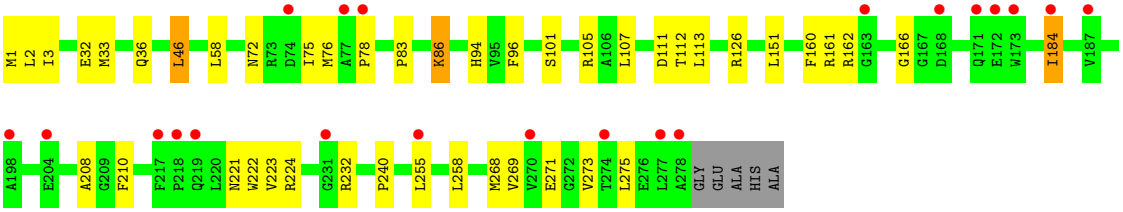




• Molecule 2: 2-heptyl-4(1H)-quinolone synthase subunit PqsB

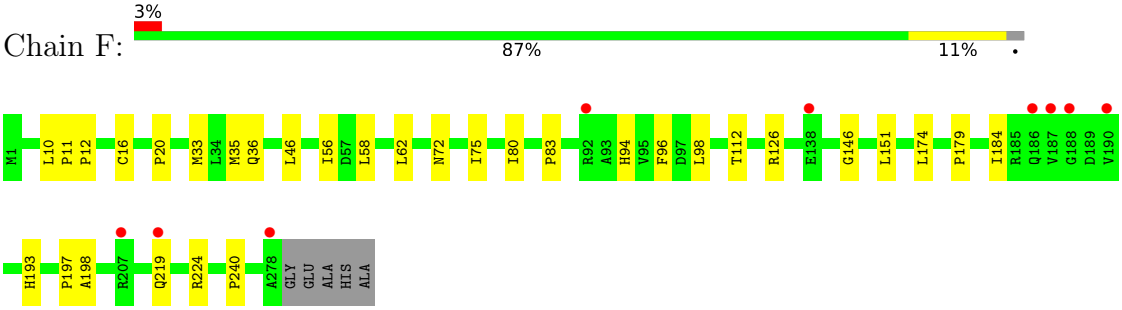
Chain D:





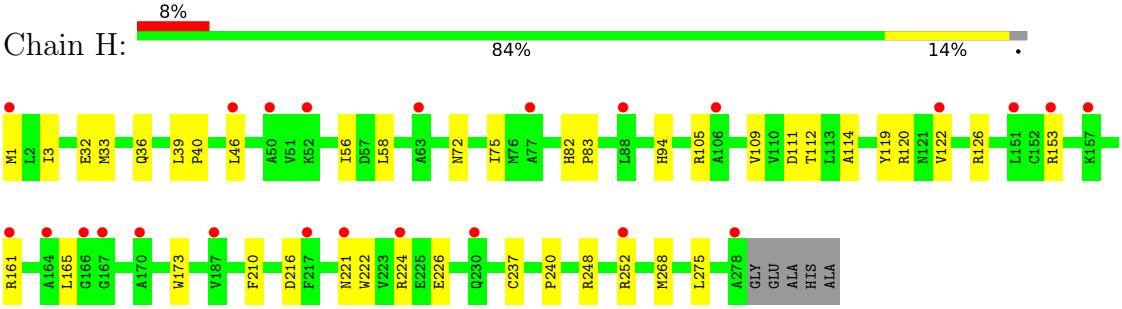
• Molecule 2: 2-heptyl-4(1H)-quinolone synthase subunit PqsB

Chain F:



• Molecule 2: 2-heptyl-4(1H)-quinolone synthase subunit PqsB

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	158.22Å 226.86Å 134.57Å 90.00° 112.33° 90.00°	Depositor
Resolution (Å)	83.84 – 2.06 83.84 – 2.06	Depositor EDS
% Data completeness (in resolution range)	50.9 (83.84-2.06) 50.9 (83.84-2.06)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 1.92Å)	Xtriage
Refinement program	PHENIX ("2.0_5936": ???)	Depositor
R, R_{free}	0.201 , 0.236 0.199 , 0.232	Depositor DCC
R_{free} test set	6961 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19912	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CL, A1J5V

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	0.19	0/2817	0.45	0/3824
1	C	0.19	0/2761	0.56	2/3749 (0.1%)
1	E	0.17	0/2771	0.42	0/3759
1	G	0.20	0/2717	0.48	1/3691 (0.0%)
2	B	0.15	0/2158	0.44	0/2932
2	D	0.19	0/2150	0.48	2/2922 (0.1%)
2	F	0.15	0/2174	0.43	0/2953
2	H	0.17	0/2157	0.43	0/2932
All	All	0.18	0/19705	0.47	5/26762 (0.0%)

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

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	221	ALA	CA-C-N	12.44	144.58	120.94
1	C	221	ALA	C-N-CA	12.44	144.58	120.94
1	G	340	GLY	N-CA-C	-5.66	108.24	115.42
2	D	184	ILE	CA-C-N	-5.53	112.63	122.42
2	D	184	ILE	C-N-CA	-5.53	112.63	122.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	339	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2753	0	2694	35	0
1	C	2701	0	2649	53	0
1	E	2710	0	2674	38	0
1	G	2657	0	2599	50	0
2	B	2117	0	2126	21	0
2	D	2109	0	2117	42	0
2	F	2133	0	2142	23	0
2	H	2116	0	2119	30	0
3	A	4	0	6	1	0
3	B	4	0	6	0	0
4	A	17	0	0	0	0
4	C	17	0	0	0	0
4	E	17	0	0	0	0
4	G	17	0	0	0	0
5	A	1	0	0	0	0
6	A	123	0	0	0	0
6	B	142	0	0	0	0
6	C	18	0	0	1	0
6	D	33	0	0	1	0
6	E	58	0	0	0	0
6	F	104	0	0	1	0
6	G	5	0	0	0	0
6	H	56	0	0	0	0
All	All	19912	0	19132	263	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 7.

All (263) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:173:TRP:HB3	2:H:268:MET:HE3	1.57	0.86
2:D:33:MET:H	2:D:36:GLN:HE21	1.25	0.81
2:F:62:LEU:HB2	2:F:126:ARG:HG3	1.67	0.74
1:G:12:GLU:HB3	1:G:177:CYS:HB2	1.68	0.74
1:E:222:LYS:HD2	2:F:184:ILE:O	1.88	0.73
1:C:226:LYS:HD2	2:D:184:ILE:O	1.89	0.72
1:A:339:THR:C	1:A:341:TRP:H	1.96	0.72
2:H:210:PHE:HD2	2:H:224:ARG:HD2	1.54	0.71
1:C:321:LEU:HD12	1:C:338:MET:SD	2.31	0.71
1:C:13:LEU:HD22	1:C:312:MET:HE1	1.73	0.70
2:H:33:MET:H	2:H:36:GLN:HE21	1.37	0.70
1:A:-6:ASN:HD21	2:F:224:ARG:NH2	1.91	0.69
2:D:273:VAL:HG13	2:D:275:LEU:HD11	1.75	0.69
2:H:210:PHE:CD2	2:H:224:ARG:HD2	2.27	0.68
2:D:162:ARG:HG3	2:D:269:VAL:HG11	1.75	0.67
1:C:201:ALA:O	2:D:86:LYS:HE3	1.95	0.66
2:B:42:VAL:HG11	2:B:88:LEU:HD11	1.77	0.65
1:E:128:GLU:HB3	1:E:338:ALA:HB1	1.78	0.65
1:C:261:MET:HE3	1:C:339:ALA:HB3	1.77	0.65
2:H:3:ILE:HD11	2:H:275:LEU:HD13	1.78	0.65
2:D:72:ASN:HB3	2:D:75:ILE:HD12	1.78	0.64
1:G:132:PHE:CG	1:G:314:PRO:HG3	2.33	0.64
1:C:343:THR:C	1:C:345:TRP:H	2.06	0.64
1:A:129(A):CYS:HB3	1:A:277:HIS:CE1	2.33	0.63
1:A:1:MET:HE1	1:A:145:GLN:HG2	1.82	0.62
1:E:203:PHE:CE2	1:E:245:MET:HB2	2.34	0.62
1:C:204:TYR:CZ	2:D:83:PRO:HG3	2.35	0.61
1:G:36:TRP:HH2	1:G:171:THR:HB	1.65	0.61
1:G:339:THR:C	1:G:341:TRP:H	2.06	0.61
2:F:72:ASN:HB3	2:F:75:ILE:HD12	1.82	0.61
1:C:43:ARG:HG3	1:C:308:ASP:HA	1.83	0.60
2:B:210:PHE:CD2	2:B:224:ARG:HD2	2.37	0.59
1:C:279:VAL:HB	1:C:338:MET:HG2	1.83	0.59
2:B:157:LYS:HZ3	2:F:219[B]:GLN:HG3	1.68	0.59
1:E:275:VAL:HB	1:E:334:MET:HG2	1.85	0.58
1:A:11:CYS:HB2	1:A:318:MET:HE1	1.86	0.58
1:C:204:TYR:HE1	2:D:78:PRO:HB2	1.68	0.58
2:D:268:MET:HA	2:D:268:MET:HE2	1.86	0.58
1:G:157:GLU:HG2	1:G:311:VAL:HG23	1.85	0.58
2:D:33:MET:H	2:D:36:GLN:NE2	2.00	0.58
1:E:244:LYS:HD3	1:E:245:MET:H	1.69	0.58
1:C:80:LEU:HD21	1:C:111:LEU:HD23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:ARG:HB2	1:E:174:ALA:HB2	1.85	0.57
1:G:204:TYR:CZ	2:H:83:PRO:HG3	2.39	0.57
1:E:339:THR:C	1:E:341:TRP:H	2.13	0.57
1:C:323:THR:HA	1:C:326:ARG:HG2	1.86	0.57
1:C:12:GLU:HG2	1:C:65:ARG:HH22	1.70	0.57
1:G:203:PHE:CE2	1:G:245:MET:HA	2.40	0.56
1:C:36:TRP:CH2	1:C:171:THR:HB	2.41	0.56
1:G:36:TRP:CH2	1:G:171:THR:HB	2.40	0.56
1:C:79:MET:HE1	1:C:142:MET:SD	2.44	0.56
1:E:89:MET:HE1	1:E:107:MET:HB2	1.87	0.56
1:E:200:ASP:O	1:E:341:TRP:HB2	2.06	0.56
1:C:121:LEU:HD11	2:D:105:ARG:HD2	1.86	0.56
2:H:33:MET:H	2:H:36:GLN:NE2	2.04	0.55
1:G:141:SER:HB3	2:H:112:THR:HG22	1.88	0.55
1:G:25:PHE:CD1	1:G:171:THR:HG22	2.41	0.55
1:G:317:LEU:HD22	1:G:334:MET:HE1	1.88	0.55
1:A:87:PRO:HD2	1:A:162:LEU:HD21	1.87	0.55
1:A:204:TYR:CE1	2:B:78:PRO:HB2	2.42	0.55
1:C:203:PHE:CD2	1:C:249:MET:HG2	2.42	0.54
2:F:126:ARG:CZ	2:F:240:PRO:HG2	2.38	0.54
1:A:128:GLU:HB3	1:A:338:ALA:HB1	1.89	0.54
1:C:25:PHE:CD1	1:C:171:THR:HG22	2.42	0.54
1:G:198:HIS:CE1	1:G:343:PHE:HB2	2.43	0.54
1:A:275:VAL:HB	1:A:334:MET:HG2	1.89	0.54
1:G:139:ALA:O	1:G:143:ILE:HD12	2.08	0.54
2:D:223:VAL:HG22	2:D:258:LEU:HD21	1.89	0.54
1:E:204:TYR:CZ	2:F:83:PRO:HG3	2.42	0.54
2:B:157:LYS:HZ3	2:F:219[B]:GLN:CG	2.20	0.54
1:G:25:PHE:HZ	1:G:44:ARG:HD2	1.73	0.54
1:C:36:TRP:HH2	1:C:171:THR:HB	1.71	0.54
2:D:221:ASN:HD22	2:D:255:LEU:HD11	1.73	0.54
2:H:72:ASN:HB3	2:H:75:ILE:HD12	1.90	0.54
1:A:157:GLU:HG2	1:A:311:VAL:HG23	1.89	0.53
1:A:339:THR:C	1:A:341:TRP:N	2.65	0.53
1:C:25:PHE:HZ	1:C:44:ARG:HD2	1.73	0.53
2:F:46:LEU:HD21	2:F:56:ILE:HD11	1.90	0.53
2:B:72:ASN:HB3	2:B:75:ILE:HD12	1.89	0.53
1:G:35:TRP:HH2	1:G:171:THR:OG1	1.91	0.53
1:G:200:ASP:O	1:G:341:TRP:HB2	2.09	0.53
1:G:270:ASP:HB3	1:G:331:ARG:HH21	1.73	0.53
1:C:159:ILE:HG21	1:C:173:PHE:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:PHE:HE2	1:E:245:MET:HB2	1.72	0.52
1:C:261:MET:HE1	1:C:280:PHE:CE1	2.44	0.52
1:E:192:LEU:HD13	1:E:348:TRP:CE2	2.44	0.52
1:C:141:SER:HB3	2:D:112:THR:HG22	1.91	0.52
2:F:46:LEU:HD23	2:F:151:LEU:HD22	1.91	0.52
1:C:204:TYR:CE1	2:D:78:PRO:HB2	2.45	0.52
1:G:300:LEU:HD22	1:G:302:MET:HE3	1.91	0.52
1:C:89:MET:O	1:C:101:GLY:HA2	2.11	0.51
1:A:200:ASP:O	1:A:341:TRP:HB2	2.09	0.51
1:G:80:LEU:HD21	1:G:111:LEU:HD23	1.92	0.51
1:C:200:ASP:O	1:C:345:TRP:HB2	2.09	0.51
1:E:157:GLU:HG2	1:E:311:VAL:HG23	1.93	0.51
1:G:79:MET:SD	1:G:142:MET:HG3	2.51	0.51
2:B:46:LEU:HD23	2:B:151:LEU:HD22	1.93	0.50
1:G:123:LEU:HD22	2:H:109:VAL:HG21	1.92	0.50
2:H:161:ARG:HE	2:H:216:ASP:HB3	1.75	0.50
2:B:9:ASN:OD1	2:B:37:ARG:HD3	2.11	0.50
1:E:82:CYS:HB3	1:E:107:MET:HE3	1.93	0.50
2:H:58:LEU:HB3	2:H:122:VAL:HG22	1.93	0.50
1:A:204:TYR:HE1	2:B:78:PRO:HB2	1.76	0.50
1:A:332:ILE:HD13	1:A:350:LEU:HD11	1.91	0.50
1:G:31:LEU:HD22	1:G:35:TRP:CZ3	2.47	0.50
2:D:166:GLY:HA3	2:D:208:ALA:HB3	1.94	0.50
1:C:12:GLU:HG3	1:C:62:ALA:HB2	1.94	0.49
2:D:160:PHE:C	2:D:161:ARG:HD2	2.36	0.49
1:E:157:GLU:HG3	1:E:309:ILE:HB	1.94	0.49
1:A:190:CYS:HA	1:A:349:GLN:O	2.13	0.49
1:C:39:TRP:O	1:C:41:VAL:HG23	2.12	0.49
2:F:20:PRO:HG2	2:F:198:ALA:HB1	1.94	0.49
3:A:401:EDO:H21	2:B:162:ARG:HD3	1.94	0.49
1:C:176:GLY:HA3	1:C:312:MET:HE2	1.94	0.49
2:D:224:ARG:HD3	2:D:224:ARG:N	2.28	0.49
1:G:121:LEU:HD11	2:H:105:ARG:HD3	1.93	0.49
1:G:157:GLU:HG3	1:G:308:MET:O	2.12	0.49
1:G:18:TYR:CE2	1:G:46:TYR:HB2	2.48	0.49
2:B:219:GLN:HG2	1:E:1:MET:HE1	1.94	0.49
1:A:43:ARG:HG3	1:A:304:ASP:HA	1.95	0.48
1:G:142:MET:HE2	2:H:112:THR:HG21	1.96	0.48
2:H:248:ARG:O	2:H:252:ARG:HG3	2.13	0.48
1:E:136:LEU:HD22	1:E:182:LEU:HD11	1.95	0.48
1:C:336:ILE:HD13	1:C:354:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:GLU:CD	1:A:205:GLU:H	2.21	0.48
1:G:192:LEU:HD12	1:G:348:TRP:CZ2	2.48	0.48
1:A:299:GLN:NE2	1:A:320:GLY:HA2	2.29	0.48
1:G:311:VAL:C	1:G:314:PRO:HD2	2.39	0.47
1:G:99:LEU:HD21	1:G:102:ARG:HD3	1.96	0.47
1:G:308:MET:HE3	1:G:308:MET:HB2	1.74	0.47
2:B:67:ASP:HB2	2:B:73:ARG:O	2.15	0.47
2:D:126:ARG:NE	2:D:240:PRO:HG2	2.30	0.47
1:G:13:LEU:HD11	1:G:308:MET:SD	2.54	0.47
2:D:58:LEU:HD11	2:D:96:PHE:CE1	2.50	0.47
1:G:163:LEU:HB3	1:G:170:SER:HB2	1.96	0.47
2:H:46:LEU:HD21	2:H:56:ILE:HD11	1.95	0.47
2:H:222:TRP:CZ3	2:H:224:ARG:HD3	2.49	0.47
1:E:142:MET:HE2	2:F:112:THR:HG21	1.95	0.47
1:G:82:CYS:HB3	1:G:107:MET:HE3	1.96	0.47
2:H:114:ALA:HA	2:H:119:TYR:CD2	2.50	0.47
1:C:17:SER:C	1:C:18:TYR:HD2	2.22	0.47
2:B:79:LYS:O	2:B:83:PRO:HD2	2.15	0.46
1:C:22:ASP:OD1	1:C:24:VAL:HG13	2.15	0.46
2:H:1:MET:SD	2:H:111:ASP:HB2	2.55	0.46
1:A:251:THR:O	1:A:255:ILE:HG13	2.15	0.46
1:C:226:LYS:HA	1:C:226:LYS:HD3	1.69	0.46
2:F:58:LEU:HD12	2:F:94:HIS:O	2.15	0.46
1:C:192:LEU:HD13	1:C:352:TRP:CE2	2.50	0.46
2:H:32:GLU:HA	2:H:36:GLN:HE22	1.80	0.46
2:F:10:LEU:HD23	2:F:146:GLY:HA3	1.97	0.46
2:H:114:ALA:HA	2:H:119:TYR:HD2	1.81	0.46
2:D:107:LEU:HD13	2:D:275:LEU:HD21	1.96	0.46
1:A:136:LEU:HD22	1:A:182:LEU:HD21	1.97	0.46
1:A:299:GLN:HE22	1:A:320:GLY:HA2	1.79	0.46
2:B:157:LYS:HD3	2:B:157:LYS:HA	1.72	0.46
1:G:128:GLU:HB3	1:G:338:ALA:HB1	1.97	0.46
2:D:210:PHE:HB3	2:D:222:TRP:CZ3	2.52	0.45
1:E:281:PRO:O	1:E:285:LYS:HG3	2.16	0.45
1:G:14:PRO:HG3	1:G:47:PHE:CD2	2.51	0.45
1:C:145:GLN:OE1	2:D:112:THR:HG23	2.16	0.45
2:D:1:MET:HE2	2:D:111:ASP:HB2	1.98	0.45
1:A:12:GLU:HG2	1:A:58:LEU:HB3	1.98	0.45
1:A:247:SER:C	1:A:250:PRO:HD2	2.42	0.45
1:A:252:ASN:HA	1:A:255:ILE:HG13	1.98	0.45
1:C:321:LEU:C	1:C:321:LEU:HD23	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:ILE:HD11	2:D:275:LEU:CD2	2.46	0.45
2:D:101:SER:HA	2:D:105:ARG:NH2	2.32	0.45
1:E:198:HIS:HB3	1:E:259[B]:ARG:HH12	1.82	0.45
1:G:278:GLN:HB3	1:G:302:MET:HE2	1.98	0.45
2:B:210:PHE:HD2	2:B:224:ARG:HD2	1.80	0.44
1:C:10:THR:HG22	1:C:66:LEU:HD12	1.98	0.44
1:E:129(A):CYS:SG	1:E:309:ILE:HA	2.57	0.44
1:E:282:PHE:CE1	1:E:283:LEU:HD22	2.52	0.44
2:F:174:LEU:HD23	2:F:197:PRO:HG2	1.98	0.44
1:E:332:ILE:HD13	1:E:350:LEU:HD11	2.00	0.44
1:C:157:GLU:CD	1:C:313:ILE:HB	2.43	0.44
2:F:58:LEU:HD11	2:F:96:PHE:CE1	2.52	0.44
2:H:32:GLU:HA	2:H:36:GLN:NE2	2.32	0.44
1:A:338:ALA:O	1:A:341:TRP:HA	2.18	0.44
1:C:-2:GLN:HA	2:H:221:ASN:HD22	1.82	0.44
1:C:142:MET:HE2	2:D:112:THR:HG21	2.00	0.44
2:D:32:GLU:HA	2:D:36:GLN:HE22	1.83	0.44
1:E:204:TYR:CE2	2:F:83:PRO:HG3	2.53	0.43
2:B:232:ARG:HA	2:B:232:ARG:HD2	1.77	0.43
1:C:13:LEU:HD11	1:C:319:TYR:CE1	2.52	0.43
1:C:103:LEU:HD22	2:D:76:MET:HE1	2.00	0.43
1:C:346:GLY:HA3	6:D:301:HOH:O	2.18	0.43
2:D:32:GLU:HA	2:D:36:GLN:NE2	2.34	0.43
1:G:275:VAL:O	1:G:334:MET:HA	2.18	0.43
1:A:67:LEU:HD12	1:A:72:THR:HB	2.00	0.43
1:E:99:LEU:HD23	1:E:99:LEU:HA	1.82	0.43
2:F:16:CYS:HB2	6:F:332:HOH:O	2.19	0.43
1:G:22:ASP:HB3	1:G:24:VAL:HG12	2.01	0.43
1:C:44:ARG:HB2	1:C:174:ALA:HB2	2.00	0.43
1:C:152:LEU:HD12	1:C:152:LEU:HA	1.85	0.43
2:D:160:PHE:O	2:D:161:ARG:HD2	2.18	0.43
1:E:36:TRP:CH2	1:E:171:THR:HB	2.54	0.43
1:E:79:MET:SD	1:E:142:MET:HG3	2.58	0.43
1:G:203:PHE:CZ	1:G:245:MET:HA	2.54	0.43
1:C:100:ARG:O	1:C:101:GLY:C	2.61	0.43
2:F:62:LEU:HD21	2:F:98:LEU:HB2	2.01	0.43
1:G:40:GLY:H	1:G:281:PRO:HD3	1.84	0.43
2:D:221:ASN:ND2	2:D:255:LEU:HD11	2.33	0.43
2:H:126:ARG:HE	2:H:240:PRO:HG2	1.83	0.43
1:G:222:LYS:HB3	1:G:223:PRO:HD3	2.01	0.43
2:H:120:ARG:O	2:H:153:ARG:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:LEU:HD23	1:E:31:LEU:HA	1.81	0.43
2:F:179:PRO:HD2	2:F:193:HIS:O	2.19	0.43
2:D:58:LEU:HD12	2:D:94:HIS:O	2.19	0.42
2:B:56:ILE:HD13	2:B:123:LEU:HD12	2.01	0.42
1:C:31:LEU:HD12	1:C:31:LEU:HA	1.93	0.42
1:A:25:PHE:CD1	1:A:171:THR:HG22	2.54	0.42
1:G:47:PHE:CE2	1:G:58:LEU:HD12	2.54	0.42
2:H:165:LEU:HD12	2:H:173:TRP:CD1	2.54	0.42
1:A:29:PRO:HB2	1:A:30:ASP:OD2	2.19	0.42
1:E:139:ALA:HB3	1:E:182:LEU:HD12	2.00	0.42
1:G:85:SER:HA	1:G:126:GLN:NE2	2.34	0.42
2:D:3:ILE:HD11	2:D:275:LEU:HD23	2.02	0.42
2:H:226:GLU:O	2:H:237:CYS:HB2	2.20	0.42
1:C:82:CYS:HB3	1:C:107:MET:HE3	2.02	0.42
2:H:82:HIS:HB2	2:H:83:PRO:HD3	2.02	0.42
1:C:79:MET:HE3	1:C:79:MET:HB2	1.70	0.42
1:E:245:MET:C	1:E:247:SER:H	2.27	0.42
1:G:-5:LEU:N	1:G:-5:LEU:HD23	2.35	0.42
1:E:248:PHE:CZ	1:E:341:TRP:HB3	2.54	0.42
1:G:275:VAL:HB	1:G:334:MET:HG2	2.02	0.42
2:D:58:LEU:HD11	2:D:96:PHE:HE1	1.85	0.42
2:H:39:LEU:HB3	2:H:40:PRO:HD3	2.02	0.42
2:B:39:LEU:HB3	2:B:40:PRO:HD3	2.02	0.41
1:C:160:SER:HA	1:C:163:LEU:HG	2.02	0.41
2:D:105:ARG:HD3	2:D:271:GLU:OE2	2.20	0.41
2:B:98:LEU:HD23	2:B:98:LEU:HA	1.83	0.41
1:C:60:VAL:HG23	1:C:115:LEU:HD21	2.02	0.41
1:C:92:ALA:HB1	1:C:110:VAL:HG11	2.02	0.41
2:F:35:MET:HE2	2:F:80:ILE:HD11	2.00	0.41
1:A:203:PHE:CG	1:A:245:MET:HG2	2.55	0.41
2:D:221:ASN:HB3	1:G:-3:PHE:O	2.20	0.41
1:C:115:LEU:HB2	1:C:117:LEU:HD13	2.01	0.41
1:G:89:MET:HE2	1:G:89:MET:HB3	1.89	0.41
1:A:204:TYR:CE1	2:B:83:PRO:HD3	2.56	0.41
2:D:126:ARG:NH1	2:D:126:ARG:HG3	2.35	0.41
1:E:222:LYS:HD3	1:E:222:LYS:HA	1.86	0.41
2:H:58:LEU:HD12	2:H:94:HIS:O	2.21	0.41
1:G:39:TRP:CE3	1:G:280:ALA:HB2	2.55	0.41
1:E:89:MET:O	1:E:101:GLY:HA2	2.20	0.41
1:E:203:PHE:CZ	1:E:245:MET:HB2	2.56	0.41
1:A:12:GLU:HB3	1:A:177:CYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.94	0.41
2:D:232:ARG:HD2	2:D:232:ARG:HA	1.86	0.41
1:E:22:ASP:OD1	1:E:24:VAL:HG13	2.20	0.41
2:D:46:LEU:HD12	2:D:151:LEU:HD22	2.02	0.41
2:F:11:PRO:HA	2:F:12:PRO:HD3	1.96	0.41
1:A:61:ARG:HG3	6:C:505:HOH:O	2.20	0.40
1:A:121:LEU:HD11	2:B:105:ARG:HD3	2.03	0.40
1:A:316:THR:HA	1:A:319:THR:HG22	2.03	0.40
1:E:199:SER:HA	1:E:342:GLY:HA2	2.04	0.40
1:E:251:THR:O	1:E:254:PRO:HG2	2.22	0.40
2:F:33:MET:O	2:F:36:GLN:HG3	2.22	0.40
1:G:257:MET:HG2	1:G:333:VAL:HG11	2.04	0.40
1:G:321:LEU:C	1:G:323:GLU:H	2.29	0.40
2:D:2:LEU:HD23	2:D:3:ILE:C	2.46	0.40
2:D:113:LEU:HD23	2:D:113:LEU:C	2.47	0.40
1:E:217:PRO:HB2	1:E:221:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	352/365 (96%)	336 (96%)	14 (4%)	2 (1%)	21 13
1	C	347/365 (95%)	333 (96%)	9 (3%)	5 (1%)	9 3
1	E	346/365 (95%)	331 (96%)	14 (4%)	1 (0%)	36 30
1	G	340/365 (93%)	328 (96%)	11 (3%)	1 (0%)	36 30
2	B	277/283 (98%)	272 (98%)	5 (2%)	0	100 100
2	D	276/283 (98%)	269 (98%)	7 (2%)	0	100 100
2	F	278/283 (98%)	273 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	277/283 (98%)	274 (99%)	3 (1%)	0	100 100
All	All	2493/2592 (96%)	2416 (97%)	68 (3%)	9 (0%)	30 23

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	40	GLY
1	C	101	GLY
1	C	221	ALA
1	A	309	ILE
1	C	250	ALA
1	C	313	ILE
1	E	309	ILE
1	G	309	ILE
1	A	246	ALA

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	291/300 (97%)	291 (100%)	0	100 100
1	C	286/300 (95%)	283 (99%)	3 (1%)	68 71
1	E	287/300 (96%)	284 (99%)	3 (1%)	68 71
1	G	281/300 (94%)	273 (97%)	8 (3%)	38 34
2	B	221/223 (99%)	221 (100%)	0	100 100
2	D	220/223 (99%)	218 (99%)	2 (1%)	70 74
2	F	223/223 (100%)	223 (100%)	0	100 100
2	H	221/223 (99%)	221 (100%)	0	100 100
All	All	2030/2092 (97%)	2014 (99%)	16 (1%)	73 77

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	-5	LEU
1	C	272	SER
1	C	321	LEU
2	D	46	LEU
2	D	86	LYS
1	E	6	LEU
1	E	126	GLN
1	E	283	LEU
1	G	-5	LEU
1	G	57	SER
1	G	70	SER
1	G	181	LEU
1	G	193	LEU
1	G	262	GLU
1	G	283	LEU
1	G	304	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-9	HIS
1	A	-6	ASN
1	A	126	GLN
1	A	299	GLN
2	B	171	GLN
2	B	251	GLN
1	C	20	ASN
1	C	126	GLN
2	D	4	GLN
2	D	36	GLN
2	D	82	HIS
2	F	82	HIS
2	F	91	ASN
2	F	230	GLN
1	G	109	ASN
2	H	36	GLN
2	H	91	ASN
2	H	121	ASN
2	H	195	ASN
2	H	221	ASN
2	H	251	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	EDO	B	301	-	3,3,3	0.26	0	2,2,2	0.29	0
3	EDO	A	401	-	3,3,3	0.26	0	2,2,2	0.29	0
4	A1J5V	A	402	1	18,18,19	0.28	0	25,25,26	0.44	0
4	A1J5V	C	401	1	18,18,19	0.22	0	25,25,26	0.38	0
4	A1J5V	G	401	1	18,18,19	0.21	0	25,25,26	0.30	0
4	A1J5V	E	401	1	18,18,19	0.23	0	25,25,26	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	301	-	-	0/1/1/1	-
3	EDO	A	401	-	-	1/1/1/1	-
4	A1J5V	A	402	1	-	2/8/8/10	0/2/2/2
4	A1J5V	C	401	1	-	2/8/8/10	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1J5V	G	401	1	-	2/8/8/10	0/2/2/2
4	A1J5V	E	401	1	-	2/8/8/10	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

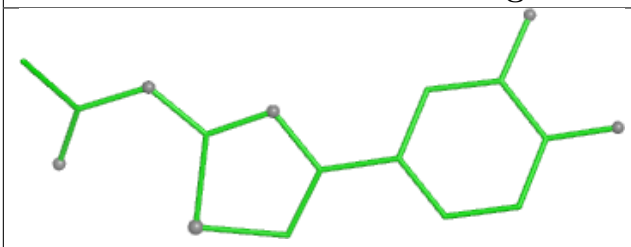
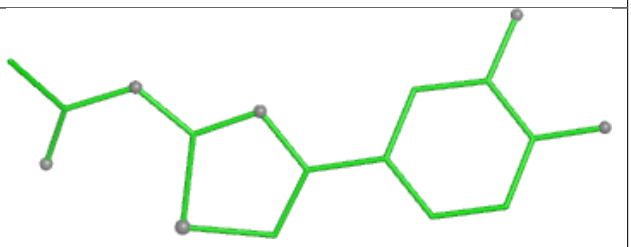
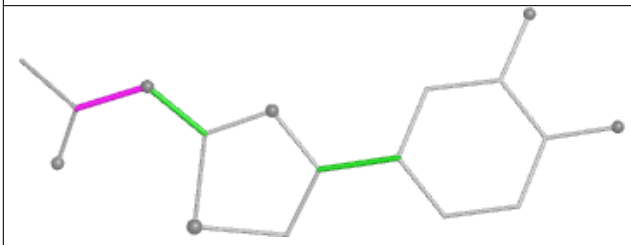
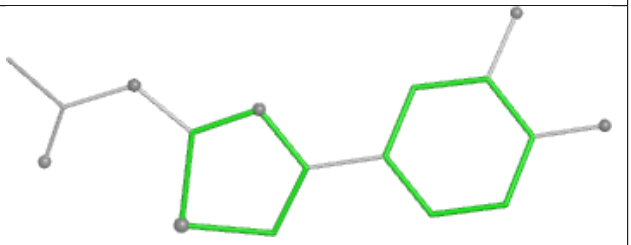
Mol	Chain	Res	Type	Atoms
4	A	402	A1J5V	C17-C16-N15-C14
4	A	402	A1J5V	O19-C16-N15-C14
4	C	401	A1J5V	C17-C16-N15-C14
4	C	401	A1J5V	O19-C16-N15-C14
4	E	401	A1J5V	C17-C16-N15-C14
4	E	401	A1J5V	O19-C16-N15-C14
4	G	401	A1J5V	C17-C16-N15-C14
4	G	401	A1J5V	O19-C16-N15-C14
3	A	401	EDO	O1-C1-C2-O2

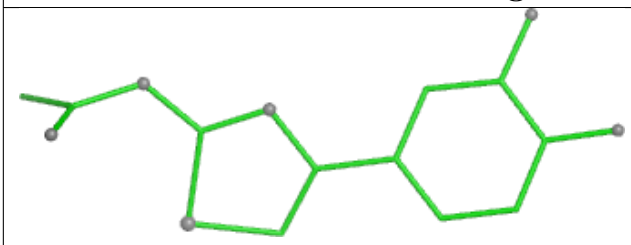
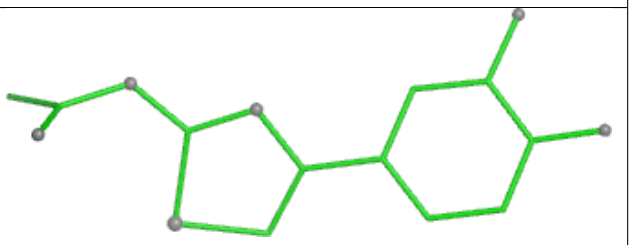
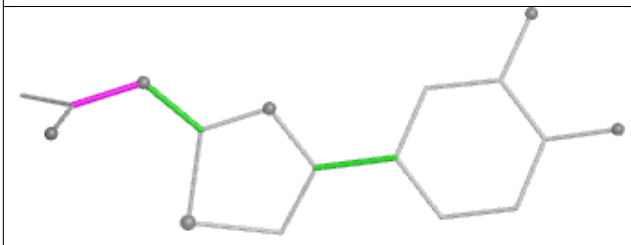
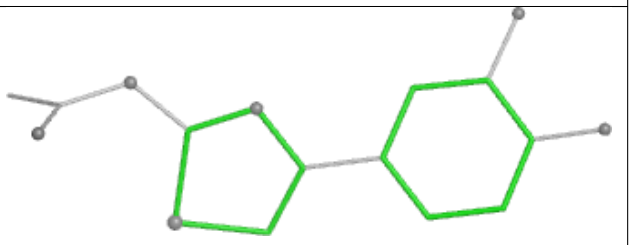
There are no ring outliers.

1 monomer is involved in 1 short contact:

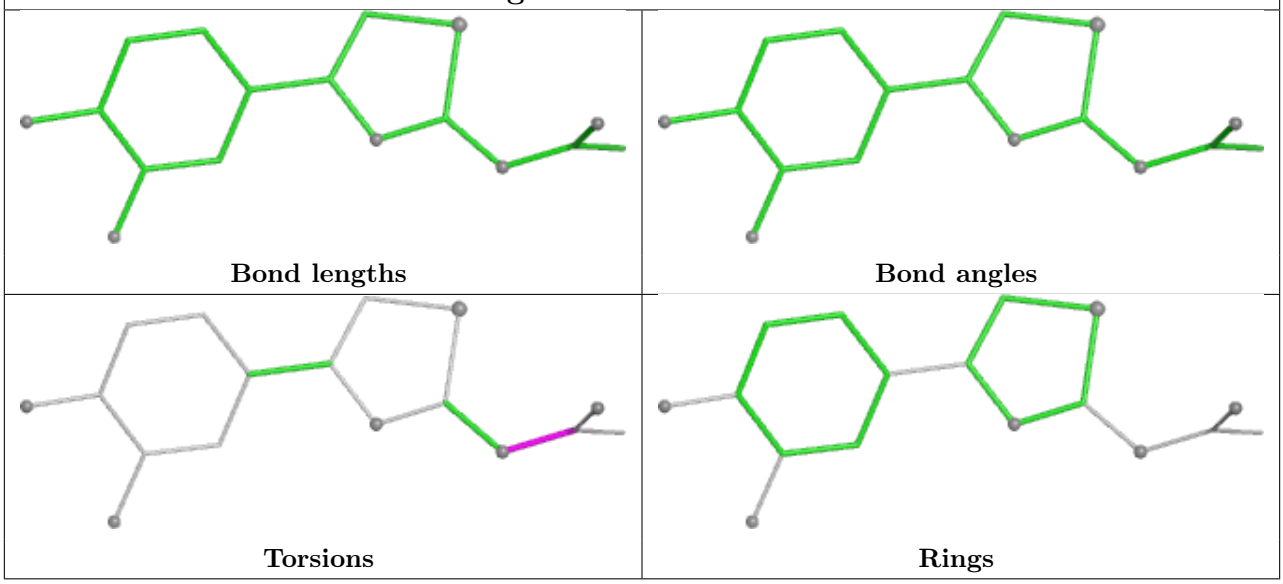
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	EDO	1	0

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

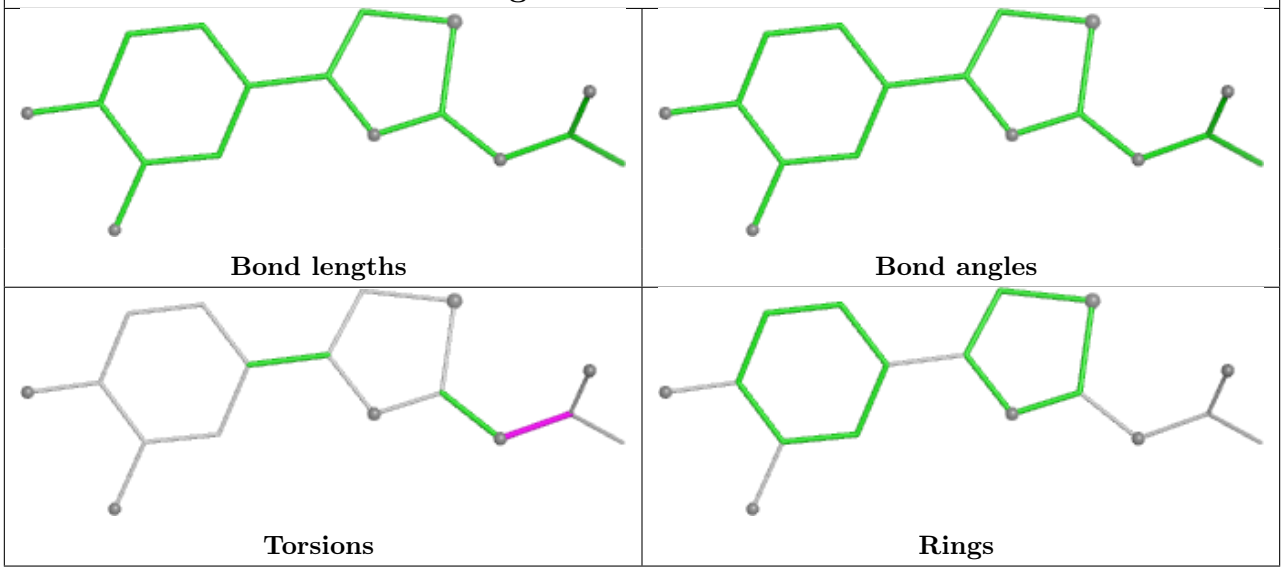
Ligand A1J5V A 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1J5V C 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand A1J5V G 401



Ligand A1J5V E 401



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	354/365 (96%)	0.53	33 (9%) 14 14	15, 44, 84, 120	2 (0%)
1	C	350/365 (95%)	1.17	52 (14%) 5 5	33, 69, 107, 130	1 (0%)
1	E	349/365 (95%)	0.63	29 (8%) 17 17	20, 54, 82, 120	2 (0%)
1	G	346/365 (94%)	1.72	115 (33%) 1 0	56, 77, 102, 127	1 (0%)
2	B	279/283 (98%)	-0.09	2 (0%) 84 86	11, 30, 56, 77	0
2	D	278/283 (98%)	1.00	21 (7%) 20 20	42, 59, 85, 115	0
2	F	278/283 (98%)	0.13	9 (3%) 50 50	14, 38, 62, 87	2 (0%)
2	H	278/283 (98%)	0.82	24 (8%) 16 17	24, 55, 79, 96	1 (0%)
All	All	2512/2592 (96%)	0.77	285 (11%) 10 10	11, 55, 93, 130	9 (0%)

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	77	ALA	10.4
2	B	77	ALA	8.4
2	H	278	ALA	6.6
1	E	340	GLY	6.5
2	F	278	ALA	6.4
1	E	246	ALA	6.4
1	A	35	TRP	6.1
1	A	-10	HIS	5.8
2	D	278	ALA	5.8
1	G	-5	LEU	5.8
1	G	245	MET	5.3
1	E	244	LYS	5.2
1	A	-9	HIS	5.0
1	C	250	ALA	5.0
1	G	204	TYR	5.0
1	E	234	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	G	35	TRP	4.9
1	C	238	PHE	4.7
1	G	218	THR	4.7
1	A	230	PHE	4.7
1	C	218	THR	4.6
1	G	345	ALA	4.5
1	A	246	ALA	4.3
1	G	322	ARG	4.3
2	D	255	LEU	4.2
2	H	230[A]	GLN	4.2
1	A	204	TYR	4.1
1	G	269	ASP	4.1
1	G	246	ALA	4.1
1	G	282	PHE	4.1
1	A	340	GLY	4.0
2	D	184	ILE	4.0
1	E	221	ALA	3.9
1	A	221	ALA	3.9
1	C	-2	GLN	3.9
1	C	205	GLU	3.8
1	A	250	PRO	3.8
1	C	-3	PHE	3.8
1	G	273	TYR	3.8
2	D	218	PRO	3.8
1	G	31	LEU	3.8
1	E	218	THR	3.7
1	G	179	VAL	3.7
1	A	0[A]	HIS	3.7
1	A	248	PHE	3.7
1	A	220	GLU	3.7
1	C	204	TYR	3.6
1	G	319	THR	3.6
1	A	341	TRP	3.5
1	C	99	LEU	3.5
1	G	340	GLY	3.5
1	A	218	THR	3.5
1	G	332	ILE	3.5
1	C	221	ALA	3.5
1	G	129(A)	CYS	3.5
1	G	353	VAL	3.4
1	A	247	SER	3.4
1	C	239	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	291	ILE	3.4
1	G	37	GLN	3.4
1	G	263	LYS	3.3
1	G	344	ALA	3.3
1	C	36	TRP	3.3
1	A	245	MET	3.3
1	C	47	PHE	3.3
1	E	37	GLN	3.3
2	D	74	ASP	3.3
1	C	176	GLY	3.2
1	C	286	PHE	3.2
1	C	90	THR	3.2
1	G	0	HIS	3.2
1	E	263	LYS	3.2
1	C	-1	GLY	3.2
1	G	317	LEU	3.1
1	G	276	PHE	3.1
1	G	50	ARG	3.1
2	H	157	LYS	3.1
1	G	354	LEU	3.1
1	G	39	TRP	3.1
1	C	231	PHE	3.1
1	E	229	LEU	3.1
1	G	13	LEU	3.1
1	A	36	TRP	3.0
1	G	348	TRP	3.0
1	C	148	ALA	3.0
1	G	326	ILE	3.0
1	G	18	TYR	3.0
1	C	227	PRO	3.0
1	C	226	LYS	3.0
2	H	122	VAL	3.0
1	G	265	GLY	3.0
1	G	279	PRO	3.0
1	C	27	ALA	3.0
2	H	170	ALA	2.9
1	G	28	VAL	2.9
2	B	187	VAL	2.9
1	G	287	TRP	2.9
1	A	-8	ALA	2.9
1	G	350	LEU	2.9
1	G	1	MET	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	92	ARG	2.9
1	G	235	SER	2.9
1	C	51	ASN	2.9
1	C	165	PHE	2.9
1	E	204	TYR	2.9
1	C	344	GLY	2.9
1	C	31	LEU	2.8
1	C	50	ARG	2.8
1	E	31	LEU	2.8
2	D	78	PRO	2.8
1	G	222	LYS	2.8
1	A	203	PHE	2.8
1	G	278	GLN	2.8
1	G	304	ASP	2.8
1	G	24	VAL	2.8
1	G	16	ARG	2.8
2	F	207[A]	ARG	2.8
1	G	321	LEU	2.8
1	G	355	VAL	2.8
2	H	252	ARG	2.8
1	G	30	ASP	2.8
2	D	187	VAL	2.8
2	H	161	ARG	2.7
1	A	227	PHE	2.7
1	G	248	PHE	2.7
1	C	180	ALA	2.7
1	G	301	THR	2.7
2	D	173	TRP	2.7
1	G	274	PHE	2.7
1	C	-5	LEU	2.7
1	E	-5	LEU	2.7
1	G	299	GLN	2.7
1	A	-6	ASN	2.7
1	G	151	VAL	2.7
1	G	271	ILE	2.7
1	A	34	SER	2.7
1	G	349	GLN	2.7
1	G	283	LEU	2.7
2	F	187	VAL	2.7
1	G	40	GLY	2.7
1	C	38	PHE	2.6
1	C	32	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	164	ALA	2.6
1	A	229	LEU	2.6
1	C	172	LEU	2.6
1	G	25	PHE	2.6
1	G	234	PHE	2.6
2	H	217	PHE	2.6
2	H	224	ARG	2.6
2	D	163	GLY	2.6
2	H	52	LYS	2.6
1	C	313	ILE	2.6
1	G	249	VAL	2.6
1	E	341	TRP	2.6
1	G	67	LEU	2.6
1	G	4	VAL	2.5
1	A	219	GLY	2.5
1	E	222	LYS	2.5
1	G	23	PRO	2.5
2	H	63	ALA	2.5
1	G	38	PHE	2.5
1	E	101	GLY	2.5
1	G	9	ILE	2.5
1	G	34	SER	2.5
1	G	180	ALA	2.5
2	D	204	GLU	2.5
1	E	248	PHE	2.5
1	G	343	PHE	2.5
1	G	247	SER	2.5
1	E	18	TYR	2.4
2	H	50	ALA	2.4
2	D	277	LEU	2.4
2	H	46	LEU	2.4
1	G	298	TYR	2.4
2	D	274	THR	2.4
1	G	256	ALA	2.4
1	G	229	LEU	2.4
2	H	166	GLY	2.4
1	C	25	PHE	2.4
1	C	252	PHE	2.4
1	E	26	ALA	2.4
1	G	8	ALA	2.4
2	F	190	VAL	2.4
1	G	316	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	289	GLU	2.3
2	D	172	GLU	2.3
1	G	134	LEU	2.3
1	G	261	LEU	2.3
2	F	219[A]	GLN	2.3
2	H	151	LEU	2.3
1	C	16	ARG	2.3
1	G	227	PHE	2.3
1	A	244	LYS	2.3
1	G	314	PRO	2.3
1	G	293	ALA	2.3
2	H	77	ALA	2.3
1	G	138	LEU	2.3
2	D	231	GLY	2.3
2	F	188	GLY	2.3
1	G	142	MET	2.3
1	G	165	PHE	2.3
2	D	217	PHE	2.3
1	C	60	VAL	2.3
1	G	275	VAL	2.3
1	A	51	ASN	2.3
1	C	360	CYS	2.3
1	G	27	ALA	2.3
1	G	172	LEU	2.3
1	G	90	THR	2.2
1	A	21	ASP	2.2
1	A	31	LEU	2.2
1	C	46	TYR	2.2
2	D	219	GLN	2.2
1	A	343	PHE	2.2
1	E	25	PHE	2.2
1	G	285	LYS	2.2
1	G	313	ILE	2.2
2	H	1	MET	2.2
1	E	201	ALA	2.2
1	E	220	GLU	2.2
1	A	223	PRO	2.2
1	E	188	ASP	2.2
1	C	110	VAL	2.2
1	C	233	LEU	2.2
1	G	103	LEU	2.2
1	G	152	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	100	ARG	2.2
1	C	74	PRO	2.1
1	G	281	PRO	2.1
1	G	-3	PHE	2.1
1	A	24	VAL	2.1
1	G	284	VAL	2.1
2	H	187	VAL	2.1
1	E	45	GLY	2.1
2	D	171	GLN	2.1
1	G	196	ALA	2.1
1	C	117	LEU	2.1
2	H	88	LEU	2.1
2	H	153	ARG	2.1
1	C	312	MET	2.1
2	D	168	ASP	2.1
1	A	217	PRO	2.1
1	C	35	TRP	2.1
1	G	88	ILE	2.1
1	G	59	VAL	2.1
1	E	50	ARG	2.1
1	G	62	ALA	2.1
1	G	69	SER	2.1
1	C	169	THR	2.1
1	G	126	GLN	2.1
2	F	186	GLN	2.1
1	E	219	GLY	2.1
1	E	342	GLY	2.1
1	G	320	GLY	2.1
1	G	36	TRP	2.1
1	A	41	VAL	2.1
1	G	95	VAL	2.1
1	G	347	VAL	2.1
1	G	73	ALA	2.1
2	H	106	ALA	2.1
1	G	70	SER	2.1
1	C	157	GLU	2.1
2	H	221	ASN	2.1
1	C	171	THR	2.1
1	G	72	THR	2.1
1	C	346	GLY	2.1
1	C	95	VAL	2.1
1	E	165	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	345	TRP	2.1
1	G	318	MET	2.0
2	F	138	GLU	2.0
1	G	168	ARG	2.0
1	G	10	THR	2.0
1	C	24	VAL	2.0
1	E	28	VAL	2.0
2	D	270	VAL	2.0
1	C	249	MET	2.0
1	G	194	ALA	2.0
1	G	288	ALA	2.0
2	D	198	ALA	2.0
1	G	193	LEU	2.0
1	G	272	ASP	2.0
1	G	5	LYS	2.0
1	G	45	GLY	2.0
2	H	167	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 oligosaccharides 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
4	A1J5V	G	401	17/18	0.83	0.25	66,84,98,99	17
4	A1J5V	A	402	17/18	0.90	0.15	43,65,77,78	0
4	A1J5V	C	401	17/18	0.90	0.14	60,75,90,90	0
3	EDO	A	401	4/4	0.90	0.15	34,49,56,65	0
4	A1J5V	E	401	17/18	0.91	0.14	39,58,70,83	17
3	EDO	B	301	4/4	0.92	0.11	38,44,45,46	0

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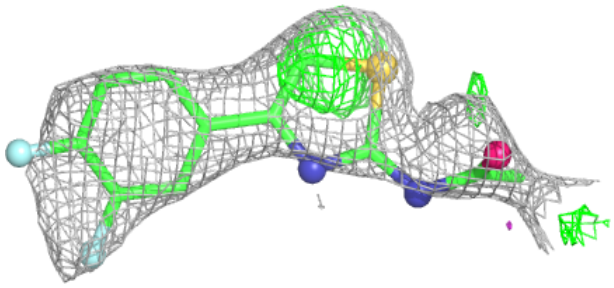
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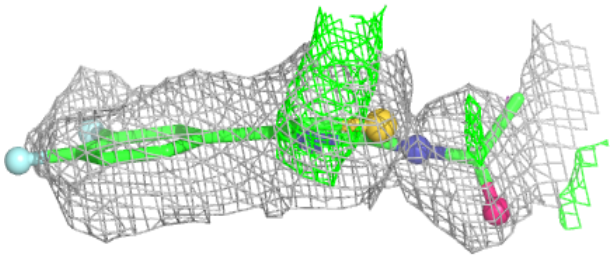
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	A	403	1/1	0.95	0.07	34,34,34,34	0

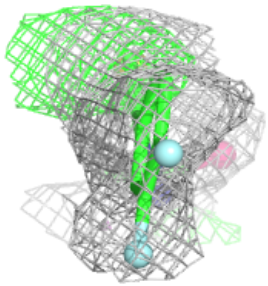
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1J5V G 401:

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

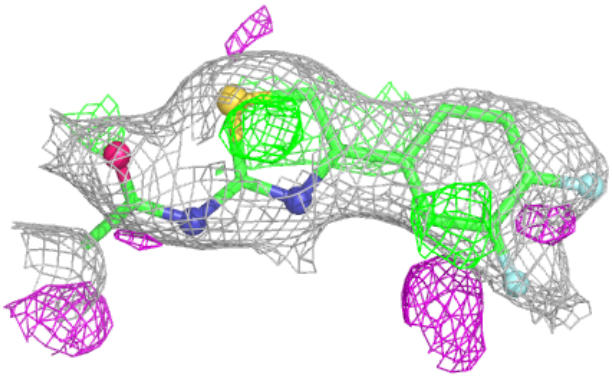


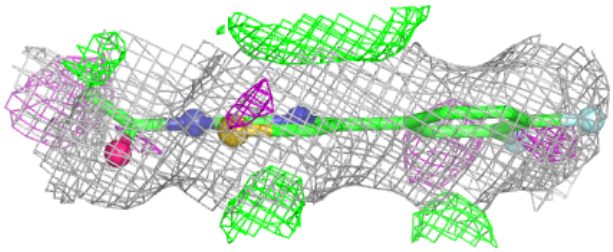


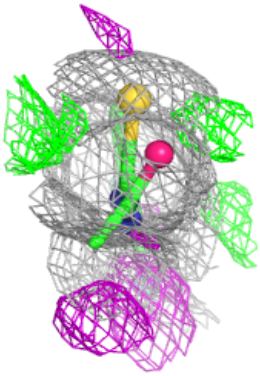


Electron density around A1J5V A 402:

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

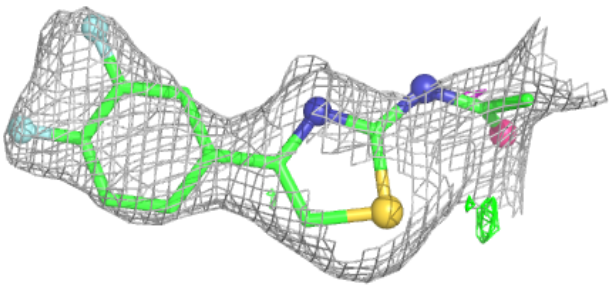


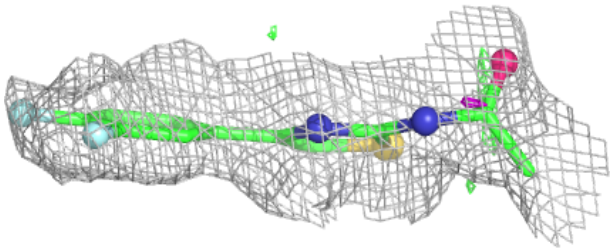


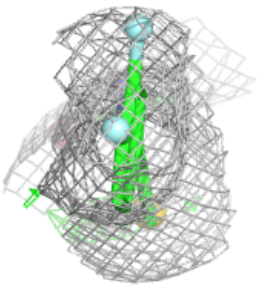


Electron density around A1J5V C 401:

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

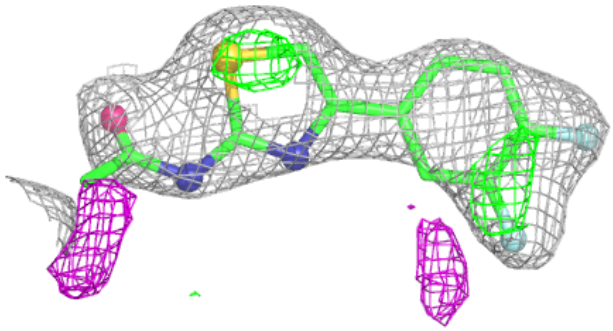


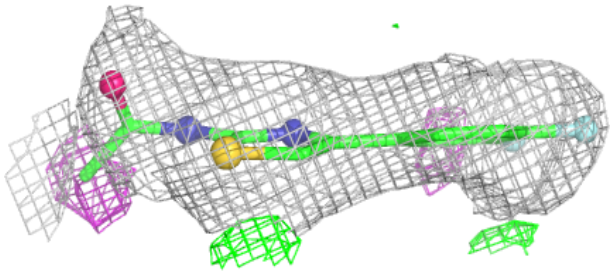


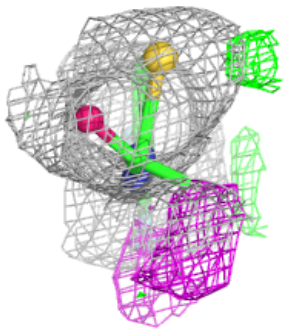


Electron density around A1J5V E 401:

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







6.5 Other polymers

There are no such residues in this entry.