Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2026 – 03:27 pm GMT

PDB ID	:	31HD / pdb_000031hd
Title	:	Crystal structure of S. aureus HMG-CoA synthase covalently bound to inhibitor
Authors	:	Gote, T.A.; van der Voort, S.P.; Overkleeft, H.S.; Hacker, S.M.; Armstrong, Z.
Deposited on	:	2026-06-04
Resolution	:	2.05 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:

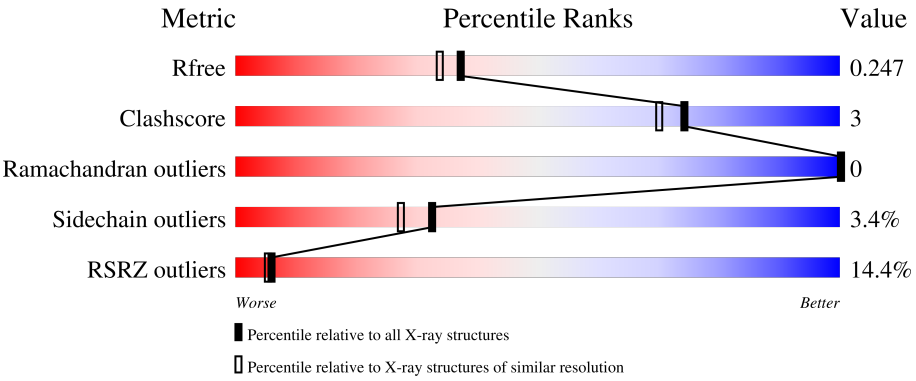
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.05 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.



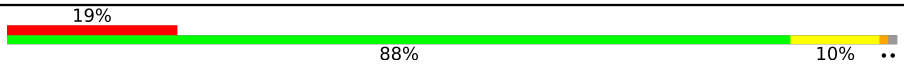
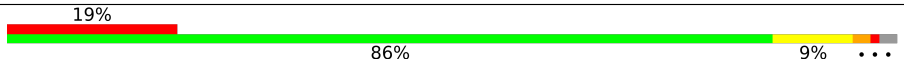
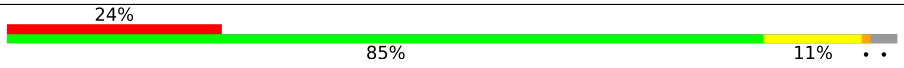
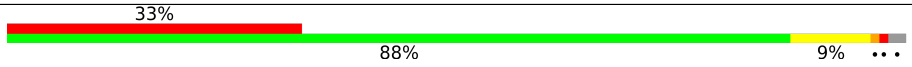
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	395	4% 89% 10% ·
1	B	395	4% 90% 8% ·
1	C	395	4% 90% 8% ··
1	D	395	6% 86% 10% · ·

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Mol	Chain	Length	Quality of chain
1	E	395	
1	F	395	
1	G	395	
1	H	395	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24723 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 Hydroxymethylglutaryl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3091	1954	523	604	10			
1	B	395	Total	C	N	O	S	0	0	0
			3099	1959	524	606	10			
1	C	390	Total	C	N	O	S	0	0	0
			3058	1935	512	601	10			
1	D	387	Total	C	N	O	S	0	0	0
			3013	1909	505	589	10			
1	E	390	Total	C	N	O	S	0	0	0
			3027	1918	509	590	10			
1	F	386	Total	C	N	O	S	0	0	0
			3030	1916	509	595	10			
1	G	384	Total	C	N	O	S	0	0	0
			3006	1904	505	587	10			
1	H	386	Total	C	N	O	S	0	0	0
			3010	1906	505	589	10			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	389	ALA	-	expression tag	UNP A0A0H2XFD1
A	390	ALA	-	expression tag	UNP A0A0H2XFD1
A	391	ALA	-	expression tag	UNP A0A0H2XFD1
A	392	LEU	-	expression tag	UNP A0A0H2XFD1
A	393	GLU	-	expression tag	UNP A0A0H2XFD1
A	394	HIS	-	expression tag	UNP A0A0H2XFD1
A	395	HIS	-	expression tag	UNP A0A0H2XFD1
A	396	HIS	-	expression tag	UNP A0A0H2XFD1
B	389	ALA	-	expression tag	UNP A0A0H2XFD1
B	390	ALA	-	expression tag	UNP A0A0H2XFD1
B	391	ALA	-	expression tag	UNP A0A0H2XFD1
B	392	LEU	-	expression tag	UNP A0A0H2XFD1
B	393	GLU	-	expression tag	UNP A0A0H2XFD1

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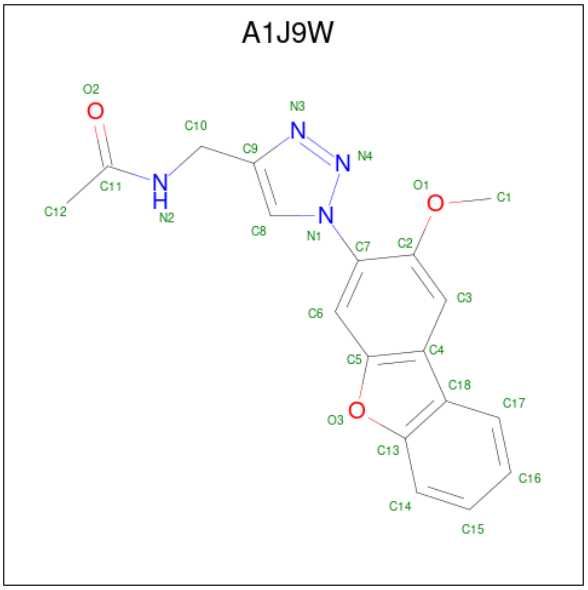
Chain	Residue	Modelled	Actual	Comment	Reference
B	394	HIS	-	expression tag	UNP A0A0H2XFD1
B	395	HIS	-	expression tag	UNP A0A0H2XFD1
B	396	HIS	-	expression tag	UNP A0A0H2XFD1
C	389	ALA	-	expression tag	UNP A0A0H2XFD1
C	390	ALA	-	expression tag	UNP A0A0H2XFD1
C	391	ALA	-	expression tag	UNP A0A0H2XFD1
C	392	LEU	-	expression tag	UNP A0A0H2XFD1
C	393	GLU	-	expression tag	UNP A0A0H2XFD1
C	394	HIS	-	expression tag	UNP A0A0H2XFD1
C	395	HIS	-	expression tag	UNP A0A0H2XFD1
C	396	HIS	-	expression tag	UNP A0A0H2XFD1
D	389	ALA	-	expression tag	UNP A0A0H2XFD1
D	390	ALA	-	expression tag	UNP A0A0H2XFD1
D	391	ALA	-	expression tag	UNP A0A0H2XFD1
D	392	LEU	-	expression tag	UNP A0A0H2XFD1
D	393	GLU	-	expression tag	UNP A0A0H2XFD1
D	394	HIS	-	expression tag	UNP A0A0H2XFD1
D	395	HIS	-	expression tag	UNP A0A0H2XFD1
D	396	HIS	-	expression tag	UNP A0A0H2XFD1
E	389	ALA	-	expression tag	UNP A0A0H2XFD1
E	390	ALA	-	expression tag	UNP A0A0H2XFD1
E	391	ALA	-	expression tag	UNP A0A0H2XFD1
E	392	LEU	-	expression tag	UNP A0A0H2XFD1
E	393	GLU	-	expression tag	UNP A0A0H2XFD1
E	394	HIS	-	expression tag	UNP A0A0H2XFD1
E	395	HIS	-	expression tag	UNP A0A0H2XFD1
E	396	HIS	-	expression tag	UNP A0A0H2XFD1
F	389	ALA	-	expression tag	UNP A0A0H2XFD1
F	390	ALA	-	expression tag	UNP A0A0H2XFD1
F	391	ALA	-	expression tag	UNP A0A0H2XFD1
F	392	LEU	-	expression tag	UNP A0A0H2XFD1
F	393	GLU	-	expression tag	UNP A0A0H2XFD1
F	394	HIS	-	expression tag	UNP A0A0H2XFD1
F	395	HIS	-	expression tag	UNP A0A0H2XFD1
F	396	HIS	-	expression tag	UNP A0A0H2XFD1
G	389	ALA	-	expression tag	UNP A0A0H2XFD1
G	390	ALA	-	expression tag	UNP A0A0H2XFD1
G	391	ALA	-	expression tag	UNP A0A0H2XFD1
G	392	LEU	-	expression tag	UNP A0A0H2XFD1
G	393	GLU	-	expression tag	UNP A0A0H2XFD1
G	394	HIS	-	expression tag	UNP A0A0H2XFD1
G	395	HIS	-	expression tag	UNP A0A0H2XFD1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	396	HIS	-	expression tag	UNP A0A0H2XFD1
H	389	ALA	-	expression tag	UNP A0A0H2XFD1
H	390	ALA	-	expression tag	UNP A0A0H2XFD1
H	391	ALA	-	expression tag	UNP A0A0H2XFD1
H	392	LEU	-	expression tag	UNP A0A0H2XFD1
H	393	GLU	-	expression tag	UNP A0A0H2XFD1
H	394	HIS	-	expression tag	UNP A0A0H2XFD1
H	395	HIS	-	expression tag	UNP A0A0H2XFD1
H	396	HIS	-	expression tag	UNP A0A0H2XFD1

- Molecule 2 is {N}-[[1-(2-methoxydibenzofuran-3-yl)-1,2,3-triazol-4-yl]methyl]ethanamide (CCD ID: A1J9W) (formula: $C_{18}H_{16}N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	18	4	3		
2	B	1	Total	C	N	O	0	0
			25	18	4	3		
2	C	1	Total	C	N	O	0	0
			25	18	4	3		
2	D	1	Total	C	N	O	0	0
			25	18	4	3		
2	E	1	Total	C	N	O	0	0
			25	18	4	3		
2	F	1	Total	C	N	O	0	0
			25	18	4	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	N	O	0	0
			25	18	4	3		

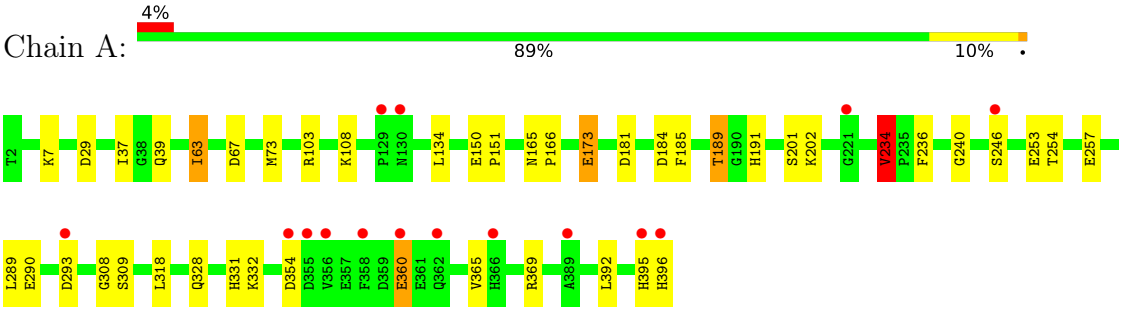
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total	O	0	0
			51	51		
3	B	51	Total	O	0	0
			51	51		
3	C	28	Total	O	0	0
			28	28		
3	D	25	Total	O	0	0
			25	25		
3	E	22	Total	O	0	0
			22	22		
3	F	15	Total	O	0	0
			15	15		
3	G	11	Total	O	0	0
			11	11		
3	H	11	Total	O	0	0
			11	11		

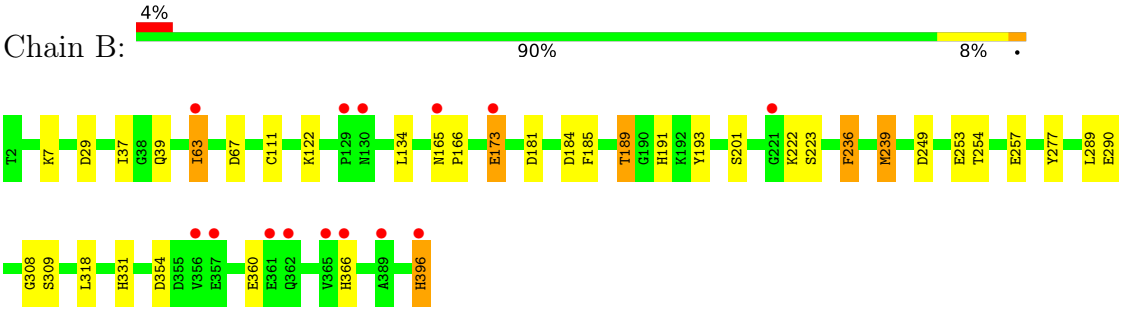
3 Residue-property plots (i)

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.

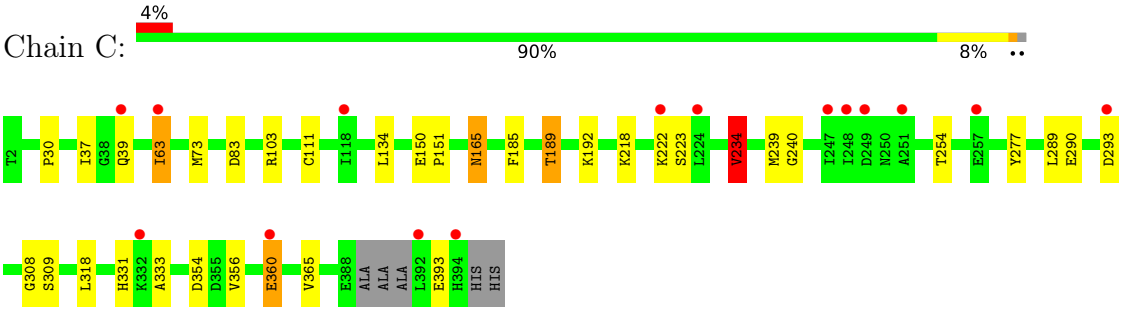
• Molecule 1: Hydroxymethylglutaryl-CoA synthase



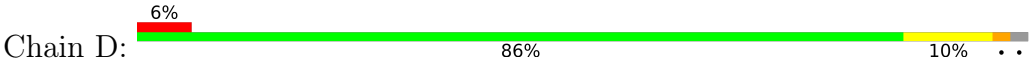
• Molecule 1: Hydroxymethylglutaryl-CoA synthase

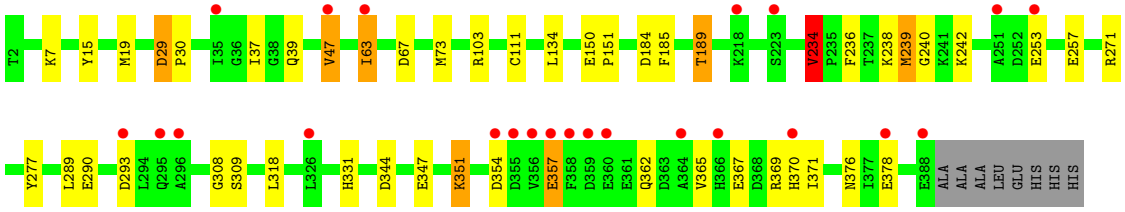


• Molecule 1: Hydroxymethylglutaryl-CoA synthase

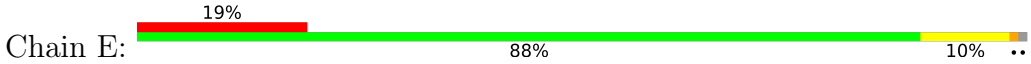


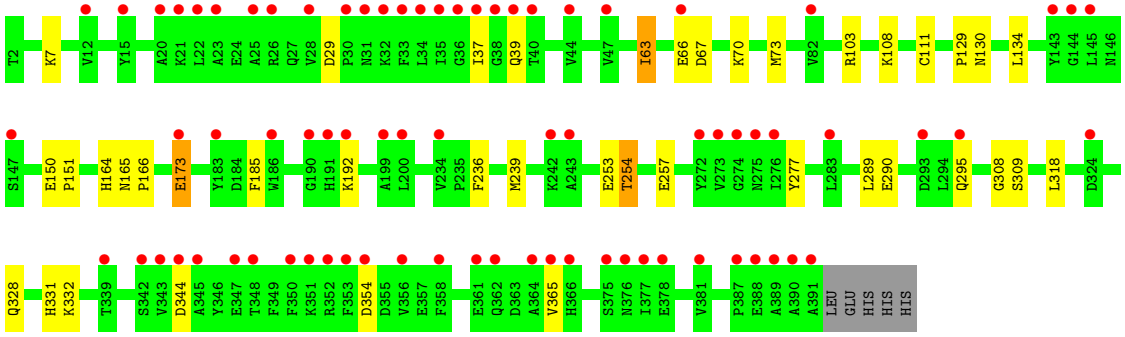
• Molecule 1: Hydroxymethylglutaryl-CoA synthase



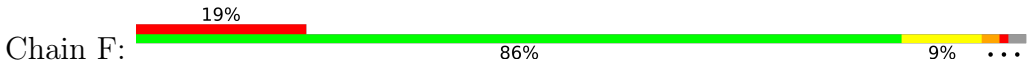


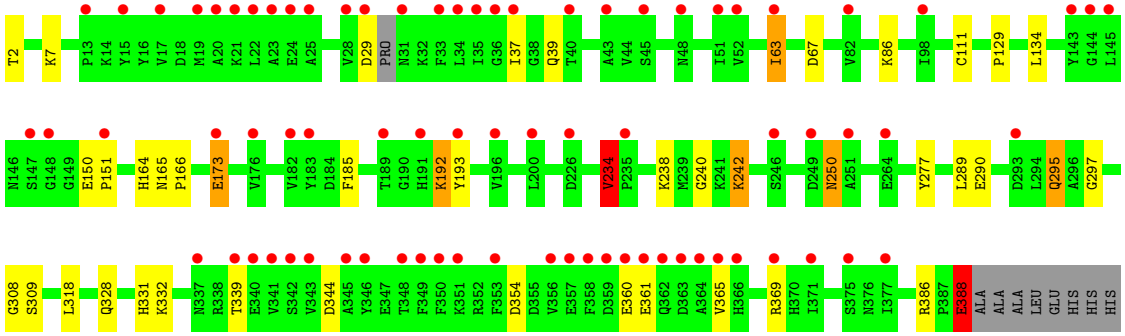
• Molecule 1: Hydroxymethylglutaryl-CoA synthase



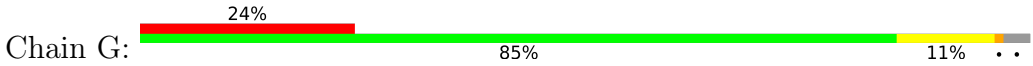


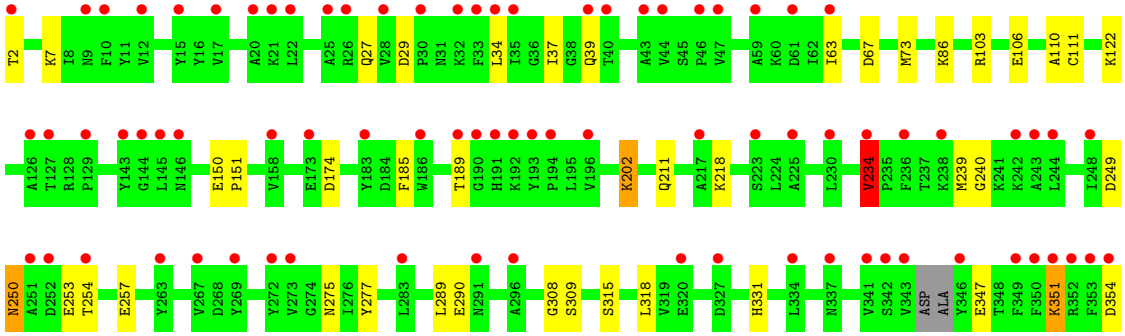
• Molecule 1: Hydroxymethylglutaryl-CoA synthase

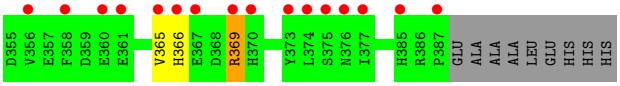




• Molecule 1: Hydroxymethylglutaryl-CoA synthase



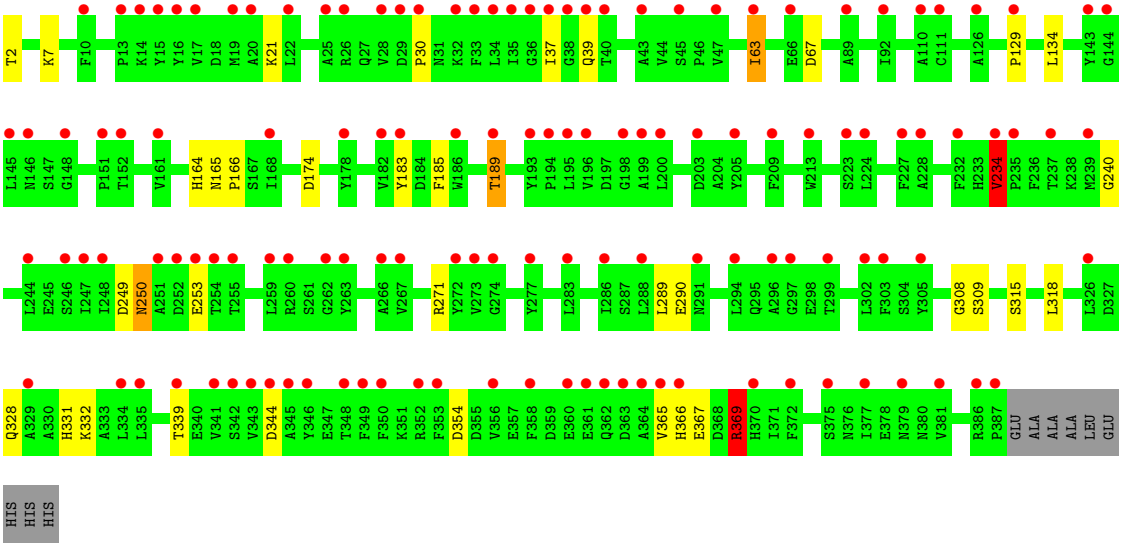




• Molecule 1: Hydroxymethylglutaryl-CoA synthase

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	178.62Å 58.13Å 194.96Å 90.00° 97.50° 90.00°	Depositor
Resolution (Å)	140.38 – 2.05 140.38 – 2.05	Depositor EDS
% Data completeness (in resolution range)	93.7 (140.38-2.05) 87.9 (140.38-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.226 , 0.250 0.226 , 0.247	Depositor DCC
R_{free} test set	11666 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24723	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.39% 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: A1J9W

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	0.68	0/3156	1.07	9/4281 (0.2%)
1	B	0.67	0/3164	1.09	9/4290 (0.2%)
1	C	0.63	0/3120	1.05	5/4229 (0.1%)
1	D	0.66	0/3075	1.11	9/4172 (0.2%)
1	E	0.59	0/3089	1.04	5/4191 (0.1%)
1	F	0.59	0/3090	1.04	9/4186 (0.2%)
1	G	0.57	0/3066	1.03	8/4155 (0.2%)
1	H	0.58	0/3072	1.04	8/4168 (0.2%)
All	All	0.62	0/24832	1.06	62/33672 (0.2%)

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	D	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	47	VAL	N-CA-CB	-12.96	88.50	110.65
1	B	173	GLU	N-CA-CB	11.16	122.85	110.35
1	E	173	GLU	CB-CG-CD	10.39	130.26	112.60
1	B	173	GLU	CB-CG-CD	8.48	127.02	112.60
1	B	254	THR	CA-CB-OG1	-7.44	98.44	109.60
1	E	173	GLU	N-CA-CB	7.33	121.27	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	388	GLU	CB-CG-CD	7.29	124.98	112.60
1	H	2	THR	CA-CB-OG1	-7.22	98.78	109.60
1	F	344	ASP	CA-CB-CG	7.09	119.69	112.60
1	B	189	THR	CA-CB-OG1	-6.98	99.13	109.60
1	D	189	THR	CA-CB-OG1	-6.92	99.22	109.60
1	A	189	THR	CA-CB-OG1	-6.91	99.24	109.60
1	F	2	THR	CA-CB-OG1	-6.79	99.42	109.60
1	C	234	VAL	N-CA-CB	-6.73	101.78	111.21
1	E	29	ASP	CA-CB-CG	6.73	119.33	112.60
1	H	249	ASP	CA-CB-CG	6.70	119.30	112.60
1	A	173	GLU	CB-CG-CD	6.62	123.86	112.60
1	A	234	VAL	N-CA-CB	-6.53	102.06	111.21
1	G	2	THR	CA-CB-OG1	-6.46	99.91	109.60
1	G	29	ASP	CA-CB-CG	6.42	119.02	112.60
1	D	29	ASP	CA-CB-CG	6.36	118.96	112.60
1	B	29	ASP	CA-CB-CG	6.34	118.94	112.60
1	G	234	VAL	N-CA-CB	-6.30	102.39	111.21
1	F	234	VAL	N-CA-CB	-6.29	102.41	111.21
1	D	234	VAL	N-CA-CB	-6.27	102.43	111.21
1	C	189	THR	CA-CB-OG1	-6.22	100.27	109.60
1	D	344	ASP	CA-CB-CG	6.20	118.80	112.60
1	D	242	LYS	CA-CB-CG	6.18	126.46	114.10
1	A	254	THR	CA-CB-OG1	-6.16	100.36	109.60
1	H	234	VAL	N-CA-CB	-6.14	102.61	111.21
1	G	249	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	29	ASP	CA-CB-CG	6.11	118.71	112.60
1	F	360	GLU	CB-CA-C	5.96	121.66	110.63
1	G	202	LYS	CB-CG-CD	5.94	124.96	111.30
1	B	236	PHE	CA-CB-CG	5.91	119.71	113.80
1	F	29	ASP	CA-CB-CG	5.84	118.44	112.60
1	D	239	MET	CG-SD-CE	-5.65	88.46	100.90
1	A	396	HIS	CA-C-O	-5.63	111.23	120.80
1	G	275	ASN	CB-CG-ND2	5.61	124.82	116.40
1	D	47	VAL	CB-CA-C	5.59	120.82	112.16
1	C	254	THR	CA-CB-OG1	-5.57	101.25	109.60
1	G	254	THR	CA-CB-OG1	-5.56	101.25	109.60
1	H	367	GLU	CB-CA-C	-5.56	98.89	109.95
1	B	239	MET	CG-SD-CE	-5.53	88.73	100.90
1	H	344	ASP	CA-CB-CG	5.48	118.08	112.60
1	E	254	THR	CA-CB-OG1	-5.45	101.43	109.60
1	C	165	ASN	CA-CB-CG	-5.40	107.20	112.60
1	A	236	PHE	CA-CB-CG	5.37	119.17	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	249	ASP	CA-CB-CG	5.32	117.92	112.60
1	D	184	ASP	CA-CB-CG	5.30	117.90	112.60
1	H	369	ARG	CG-CD-NE	5.20	123.43	112.00
1	A	181	ASP	CA-CB-CG	5.17	117.77	112.60
1	F	386	ARG	CB-CG-CD	5.16	123.16	111.30
1	E	344	ASP	CA-CB-CG	5.15	117.75	112.60
1	C	360	GLU	CB-CG-CD	5.15	121.35	112.60
1	F	339	THR	CA-CB-OG1	-5.09	101.96	109.60
1	H	189	THR	CA-CB-OG1	-5.09	101.96	109.60
1	G	189	THR	CA-CB-OG1	-5.08	101.97	109.60
1	A	369	ARG	CG-CD-NE	-5.08	100.83	112.00
1	H	339	THR	CA-CB-OG1	-5.06	102.01	109.60
1	B	181	ASP	CA-CB-CG	5.06	117.66	112.60
1	F	173	GLU	N-CA-CB	5.01	115.96	110.35

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	271	ARG	Sidechain
1	H	271	ARG	Sidechain

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	3091	0	2977	17	0
1	B	3099	0	2992	20	0
1	C	3058	0	2951	16	0
1	D	3013	0	2903	24	0
1	E	3027	0	2923	20	0
1	F	3030	0	2931	20	0
1	G	3006	0	2914	19	0
1	H	3010	0	2904	17	0
2	A	25	0	0	1	0
2	B	25	0	0	1	0
2	C	25	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	25	0	0	1	0
2	E	25	0	0	1	0
2	F	25	0	0	0	0
2	G	25	0	0	1	0
3	A	51	0	0	1	0
3	B	51	0	0	2	0
3	C	28	0	0	1	0
3	D	25	0	0	1	0
3	E	22	0	0	1	0
3	F	15	0	0	0	0
3	G	11	0	0	0	0
3	H	11	0	0	0	0
All	All	24723	0	23495	147	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (147) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLN:HE21	1:A:332:LYS:HE3	1.54	0.73
1:A:360:GLU:H	1:A:360:GLU:CD	1.98	0.71
1:B:122:LYS:NZ	1:B:173:GLU:HG2	2.09	0.66
1:C:239:MET:O	1:C:239:MET:HE3	1.96	0.65
1:G:347:GLU:O	1:G:351:LYS:HG2	2.00	0.62
1:F:369:ARG:HG2	1:F:388:GLU:HG3	1.82	0.62
1:D:357:GLU:HG3	1:D:376:ASN:HA	1.81	0.62
1:F:86:LYS:NZ	1:H:308:GLY:O	2.33	0.61
1:D:39:GLN:HB3	3:D:502:HOH:O	2.00	0.61
1:A:234:VAL:HG22	1:A:240:GLY:HA3	1.85	0.59
1:B:223:SER:HB2	3:B:538:HOH:O	2.04	0.58
1:G:211:GLN:HA	1:G:211:GLN:OE1	2.02	0.57
1:G:253:GLU:HG2	1:G:257:GLU:OE1	2.05	0.57
1:A:39:GLN:HB3	3:A:506:HOH:O	2.05	0.57
1:A:289:LEU:HD22	1:A:318:LEU:HD21	1.85	0.56
1:B:191:HIS:CE1	1:F:295:GLN:HG2	2.40	0.56
1:C:234:VAL:HG22	1:C:240:GLY:HA3	1.87	0.56
1:D:234:VAL:HG22	1:D:240:GLY:HA3	1.88	0.56
1:C:223:SER:HB2	3:C:526:HOH:O	2.05	0.56
1:E:70:LYS:HD3	1:E:130:ASN:O	2.06	0.55
1:E:290:GLU:OE1	1:E:331:HIS:ND1	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:VAL:HG22	1:G:240:GLY:HA3	1.88	0.55
1:D:290:GLU:OE1	1:D:331:HIS:ND1	2.34	0.55
1:H:289:LEU:HD22	1:H:318:LEU:HD21	1.88	0.55
1:C:333:ALA:HB1	1:D:29:ASP:HB2	1.89	0.54
1:H:234:VAL:HG22	1:H:240:GLY:HA3	1.90	0.54
1:G:289:LEU:HD22	1:G:318:LEU:HD21	1.89	0.54
1:C:290:GLU:OE1	1:C:331:HIS:ND1	2.33	0.54
1:E:39:GLN:HB3	3:E:514:HOH:O	2.07	0.54
1:F:234:VAL:HG22	1:F:240:GLY:HA3	1.90	0.54
1:F:250:ASN:HD22	1:F:250:ASN:N	2.06	0.53
1:B:290:GLU:OE1	1:B:331:HIS:ND1	2.33	0.53
1:H:369:ARG:HH11	1:H:369:ARG:HB2	1.74	0.53
1:D:253:GLU:HG2	1:D:257:GLU:OE1	2.09	0.52
1:F:289:LEU:HD22	1:F:318:LEU:HD21	1.91	0.52
1:B:289:LEU:HD22	1:B:318:LEU:HD21	1.90	0.52
1:F:328:GLN:HE21	1:F:332:LYS:HE3	1.75	0.52
1:A:290:GLU:OE1	1:A:331:HIS:ND1	2.33	0.52
1:A:253:GLU:HG2	1:A:257:GLU:OE1	2.10	0.51
1:H:366:HIS:HA	1:H:369:ARG:HH12	1.75	0.51
1:D:365:VAL:HG22	1:D:369:ARG:HH21	1.76	0.51
1:G:290:GLU:OE1	1:G:331:HIS:ND1	2.33	0.50
1:E:289:LEU:HD22	1:E:318:LEU:HD21	1.93	0.50
1:G:250:ASN:HD22	1:G:250:ASN:N	2.09	0.50
1:B:193:TYR:CE2	1:F:297:GLY:HA3	2.46	0.50
1:C:289:LEU:HD22	1:C:318:LEU:HD21	1.94	0.50
1:D:289:LEU:HD22	1:D:318:LEU:HD21	1.94	0.50
1:B:7:LYS:NZ	1:B:67:ASP:OD2	2.43	0.49
1:A:7:LYS:NZ	1:A:67:ASP:OD2	2.44	0.49
1:D:7:LYS:NZ	1:D:67:ASP:OD2	2.45	0.49
1:H:308:GLY:N	1:H:309:SER:HA	2.28	0.49
1:E:308:GLY:O	1:G:86:LYS:NZ	2.45	0.49
2:D:401:A1J9W:C8	2:D:401:A1J9W:O1	2.61	0.48
1:F:308:GLY:N	1:F:309:SER:HA	2.28	0.48
1:B:396:HIS:N	1:B:396:HIS:ND1	2.62	0.48
1:G:308:GLY:N	1:G:309:SER:HA	2.29	0.48
1:B:122:LYS:HZ1	1:B:173:GLU:HG2	1.77	0.48
1:D:308:GLY:N	1:D:309:SER:HA	2.28	0.48
1:B:39:GLN:HB3	3:B:501:HOH:O	2.14	0.47
2:B:401:A1J9W:C8	2:B:401:A1J9W:O1	2.62	0.47
1:H:290:GLU:OE1	1:H:331:HIS:ND1	2.33	0.47
1:C:308:GLY:N	1:C:309:SER:HA	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:401:A1J9W:O1	2:C:401:A1J9W:C8	2.63	0.47
1:G:110:ALA:HB1	2:G:401:A1J9W:O2	2.15	0.47
1:H:250:ASN:HD22	1:H:250:ASN:N	2.13	0.47
1:B:122:LYS:HZ3	1:B:173:GLU:HG2	1.77	0.47
1:E:328:GLN:HE21	1:E:332:LYS:HE3	1.80	0.47
1:B:308:GLY:N	1:B:309:SER:HA	2.30	0.46
2:A:401:A1J9W:C8	2:A:401:A1J9W:O1	2.64	0.46
1:H:7:LYS:NZ	1:H:67:ASP:OD2	2.45	0.46
1:D:63:ILE:HD11	1:D:134:LEU:HD22	1.97	0.46
1:G:7:LYS:NZ	1:G:67:ASP:OD2	2.45	0.46
1:C:37:ILE:HG22	1:C:39:GLN:HG2	1.97	0.46
1:D:347:GLU:O	1:D:351:LYS:HG2	2.15	0.45
1:A:308:GLY:N	1:A:309:SER:HA	2.31	0.45
1:D:367:GLU:O	1:D:370:HIS:CD2	2.69	0.45
1:D:370:HIS:ND1	1:D:371:ILE:HG23	2.32	0.45
1:E:308:GLY:N	1:E:309:SER:HA	2.30	0.45
1:D:37:ILE:HG22	1:D:39:GLN:HG2	1.98	0.45
1:C:63:ILE:HD11	1:C:134:LEU:HD22	1.98	0.45
2:E:401:A1J9W:C8	2:E:401:A1J9W:O1	2.64	0.45
1:A:108:LYS:NZ	1:C:83:ASP:O	2.40	0.45
1:D:370:HIS:CE1	1:D:371:ILE:HG23	2.52	0.45
1:B:253:GLU:HG2	1:B:257:GLU:OE1	2.16	0.45
1:B:63:ILE:HD11	1:B:134:LEU:HD22	1.98	0.45
1:C:360:GLU:H	1:C:360:GLU:CD	2.25	0.45
1:H:328:GLN:HE21	1:H:332:LYS:HE3	1.82	0.45
1:C:192:LYS:NZ	1:E:254:THR:HG23	2.32	0.45
1:F:290:GLU:OE1	1:F:331:HIS:ND1	2.33	0.45
1:A:191:HIS:CE1	1:E:295:GLN:CD	2.95	0.44
1:F:63:ILE:HD11	1:F:134:LEU:HD22	2.00	0.44
1:C:333:ALA:HB1	1:D:29:ASP:CB	2.47	0.44
1:D:19:MET:HE1	1:D:151:PRO:HB3	1.99	0.44
1:F:86:LYS:HE3	1:H:183:TYR:CZ	2.52	0.44
1:D:15:TYR:OH	1:D:362:GLN:HA	2.18	0.44
1:C:150:GLU:N	1:C:151:PRO:HD2	2.32	0.44
1:H:174:ASP:OD2	1:H:315:SER:OG	2.35	0.44
1:H:63:ILE:HD11	1:H:134:LEU:HD22	2.00	0.44
1:E:63:ILE:HD11	1:E:134:LEU:HD22	1.99	0.44
1:G:174:ASP:OD2	1:G:315:SER:OG	2.34	0.43
1:A:73:MET:HG2	1:A:103:ARG:HB2	2.01	0.43
1:E:7:LYS:NZ	1:E:67:ASP:OD2	2.47	0.43
1:E:73:MET:HG2	1:E:103:ARG:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:GLU:N	1:E:151:PRO:HD2	2.34	0.43
1:D:238:LYS:HD3	1:D:238:LYS:HA	1.39	0.43
1:F:37:ILE:HG22	1:F:39:GLN:HG2	2.01	0.43
1:A:150:GLU:N	1:A:151:PRO:HD2	2.33	0.43
1:G:366:HIS:O	1:G:369:ARG:HD3	2.19	0.43
1:D:73:MET:HG2	1:D:103:ARG:HB2	2.01	0.42
1:F:150:GLU:N	1:F:151:PRO:HD2	2.34	0.42
1:E:108:LYS:NZ	1:G:106:GLU:OE2	2.46	0.42
1:G:202:LYS:HG3	1:G:239:MET:CE	2.49	0.42
1:A:63:ILE:HD11	1:A:134:LEU:HD22	2.00	0.42
1:F:238:LYS:O	1:F:242:LYS:HG2	2.20	0.42
1:G:150:GLU:N	1:G:151:PRO:HD2	2.34	0.42
1:A:184:ASP:HB2	1:A:201:SER:HA	2.02	0.42
1:B:184:ASP:HB2	1:B:201:SER:HA	2.02	0.42
1:E:37:ILE:HG22	1:E:39:GLN:HG2	2.01	0.42
1:B:37:ILE:HG22	1:B:39:GLN:HG2	2.01	0.42
1:E:111:CYS:SG	1:E:277:TYR:HA	2.60	0.41
1:F:7:LYS:NZ	1:F:67:ASP:OD2	2.46	0.41
1:F:129:PRO:HA	1:F:164:HIS:CD2	2.56	0.41
1:C:73:MET:HG2	1:C:103:ARG:HB2	2.01	0.41
1:D:111:CYS:SG	1:D:277:TYR:HA	2.60	0.41
1:E:165:ASN:N	1:E:166:PRO:CD	2.84	0.41
1:B:236:PHE:CE2	1:B:239:MET:HB2	2.56	0.41
1:G:37:ILE:HG22	1:G:39:GLN:HG2	2.01	0.41
1:G:111:CYS:SG	1:G:277:TYR:HA	2.59	0.41
1:H:165:ASN:N	1:H:166:PRO:CD	2.82	0.41
1:F:165:ASN:N	1:F:166:PRO:CD	2.84	0.41
1:E:129:PRO:HA	1:E:164:HIS:CD2	2.56	0.41
1:H:289:LEU:CD2	1:H:318:LEU:HD21	2.51	0.41
1:D:150:GLU:HB3	1:D:151:PRO:HD3	2.02	0.41
1:D:236:PHE:CE2	1:D:239:MET:HB2	2.56	0.41
1:F:111:CYS:SG	1:F:277:TYR:HA	2.60	0.41
1:H:129:PRO:HA	1:H:164:HIS:CD2	2.55	0.41
1:A:37:ILE:HG22	1:A:39:GLN:HG2	2.03	0.41
1:B:289:LEU:CD2	1:B:318:LEU:HD21	2.50	0.41
1:H:37:ILE:HG22	1:H:39:GLN:HG2	2.02	0.41
1:F:192:LYS:HG3	1:F:193:TYR:CE2	2.56	0.40
1:E:236:PHE:CE2	1:E:239:MET:HB2	2.56	0.40
1:G:73:MET:HG2	1:G:103:ARG:HB2	2.03	0.40
1:A:165:ASN:N	1:A:166:PRO:CD	2.85	0.40
1:C:111:CYS:SG	1:C:277:TYR:HA	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:CYS:SG	1:B:277:TYR:HA	2.61	0.40
1:B:165:ASN:N	1:B:166:PRO:CD	2.85	0.40
1:E:253:GLU:HG3	1:E:257:GLU:OE1	2.21	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	393/395 (100%)	380 (97%)	13 (3%)	0	100	100
1	B	393/395 (100%)	380 (97%)	13 (3%)	0	100	100
1	C	386/395 (98%)	375 (97%)	11 (3%)	0	100	100
1	D	385/395 (98%)	369 (96%)	16 (4%)	0	100	100
1	E	388/395 (98%)	375 (97%)	13 (3%)	0	100	100
1	F	382/395 (97%)	369 (97%)	13 (3%)	0	100	100
1	G	380/395 (96%)	367 (97%)	13 (3%)	0	100	100
1	H	384/395 (97%)	371 (97%)	13 (3%)	0	100	100
All	All	3091/3160 (98%)	2986 (97%)	105 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/323 (99%)	308 (96%)	13 (4%)	28	22
1	B	323/323 (100%)	315 (98%)	8 (2%)	42	39
1	C	320/323 (99%)	307 (96%)	13 (4%)	27	21
1	D	312/323 (97%)	301 (96%)	11 (4%)	32	27
1	E	312/323 (97%)	305 (98%)	7 (2%)	45	44
1	F	317/323 (98%)	305 (96%)	12 (4%)	29	24
1	G	314/323 (97%)	302 (96%)	12 (4%)	29	24
1	H	313/323 (97%)	302 (96%)	11 (4%)	32	27
All	All	2532/2584 (98%)	2445 (97%)	87 (3%)	32	27

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ILE
1	A	173	GLU
1	A	185	PHE
1	A	189	THR
1	A	202	LYS
1	A	234	VAL
1	A	246	SER
1	A	293	ASP
1	A	354	ASP
1	A	360	GLU
1	A	365	VAL
1	A	392	LEU
1	A	395	HIS
1	B	63	ILE
1	B	185	PHE
1	B	189	THR
1	B	222	LYS
1	B	354	ASP
1	B	360	GLU
1	B	366	HIS
1	B	396	HIS
1	C	30	PRO
1	C	63	ILE
1	C	165	ASN
1	C	185	PHE
1	C	189	THR
1	C	218	LYS

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Mol	Chain	Res	Type
1	C	222	LYS
1	C	234	VAL
1	C	293	ASP
1	C	354	ASP
1	C	356	VAL
1	C	365	VAL
1	C	393	GLU
1	D	30	PRO
1	D	47	VAL
1	D	63	ILE
1	D	185	PHE
1	D	189	THR
1	D	234	VAL
1	D	293	ASP
1	D	351	LYS
1	D	354	ASP
1	D	357	GLU
1	D	378	GLU
1	E	63	ILE
1	E	66	GLU
1	E	173	GLU
1	E	185	PHE
1	E	192	LYS
1	E	354	ASP
1	E	365	VAL
1	F	63	ILE
1	F	173	GLU
1	F	185	PHE
1	F	192	LYS
1	F	234	VAL
1	F	242	LYS
1	F	250	ASN
1	F	295	GLN
1	F	354	ASP
1	F	361	GLU
1	F	365	VAL
1	F	388	GLU
1	G	27	GLN
1	G	34	LEU
1	G	63	ILE
1	G	122	LYS
1	G	185	PHE

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Mol	Chain	Res	Type
1	G	218	LYS
1	G	234	VAL
1	G	250	ASN
1	G	351	LYS
1	G	354	ASP
1	G	365	VAL
1	G	369	ARG
1	H	21	LYS
1	H	30	PRO
1	H	63	ILE
1	H	185	PHE
1	H	189	THR
1	H	234	VAL
1	H	250	ASN
1	H	253	GLU
1	H	354	ASP
1	H	365	VAL
1	H	369	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	146	ASN
1	A	191	HIS
1	A	210	GLN
1	A	328	GLN
1	A	362	GLN
1	B	210	GLN
1	B	394	HIS
1	C	172	ASN
1	C	210	GLN
1	D	210	GLN
1	E	172	ASN
1	E	210	GLN
1	E	328	GLN
1	F	172	ASN
1	F	250	ASN
1	F	328	GLN
1	G	27	GLN
1	G	165	ASN
1	G	210	GLN

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Mol	Chain	Res	Type
1	G	250	ASN
1	H	146	ASN
1	H	165	ASN
1	H	250	ASN
1	H	328	GLN
1	H	370	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	A1J9W	C	401	1	28,28,28	0.39	0	40,40,40	1.08	2 (5%)
2	A1J9W	G	401	1	28,28,28	0.34	0	40,40,40	0.91	2 (5%)
2	A1J9W	A	401	1	28,28,28	0.64	0	40,40,40	1.05	4 (10%)
2	A1J9W	F	401	1	28,28,28	0.31	0	40,40,40	0.83	2 (5%)
2	A1J9W	B	401	1	28,28,28	0.53	0	40,40,40	1.31	3 (7%)
2	A1J9W	E	401	1	28,28,28	0.37	0	40,40,40	0.73	0
2	A1J9W	D	401	1	28,28,28	0.40	0	40,40,40	0.89	1 (2%)

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	A1J9W	C	401	1	-	1/11/23/23	0/4/4/4
2	A1J9W	G	401	1	-	1/11/23/23	0/4/4/4
2	A1J9W	A	401	1	-	1/11/23/23	0/4/4/4
2	A1J9W	F	401	1	-	1/11/23/23	0/4/4/4
2	A1J9W	B	401	1	-	1/11/23/23	0/4/4/4
2	A1J9W	E	401	1	-	1/11/23/23	0/4/4/4
2	A1J9W	D	401	1	-	1/11/23/23	0/4/4/4

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	401	A1J9W	C1-O1-C2	3.58	122.94	117.53
2	B	401	A1J9W	O1-C2-C7	-3.17	111.73	116.06
2	A	401	A1J9W	C6-C5-C4	-2.97	121.88	124.46
2	B	401	A1J9W	C7-N1-N4	2.79	124.14	119.70
2	G	401	A1J9W	C6-C5-C4	-2.65	122.16	124.46
2	F	401	A1J9W	C6-C5-C4	-2.56	122.24	124.46
2	D	401	A1J9W	C6-C5-C4	-2.55	122.24	124.46
2	F	401	A1J9W	C1-O1-C2	2.39	121.14	117.53
2	B	401	A1J9W	C15-C14-C13	-2.38	115.34	119.71
2	C	401	A1J9W	C6-C7-N1	2.36	121.55	118.45
2	A	401	A1J9W	C15-C14-C13	-2.22	115.63	119.71
2	A	401	A1J9W	C9-C10-N2	-2.17	108.80	112.33
2	C	401	A1J9W	C15-C14-C13	-2.05	115.94	119.71
2	A	401	A1J9W	O1-C2-C7	-2.01	113.31	116.06

There are no chirality outliers.

All (7) torsion outliers are listed below:

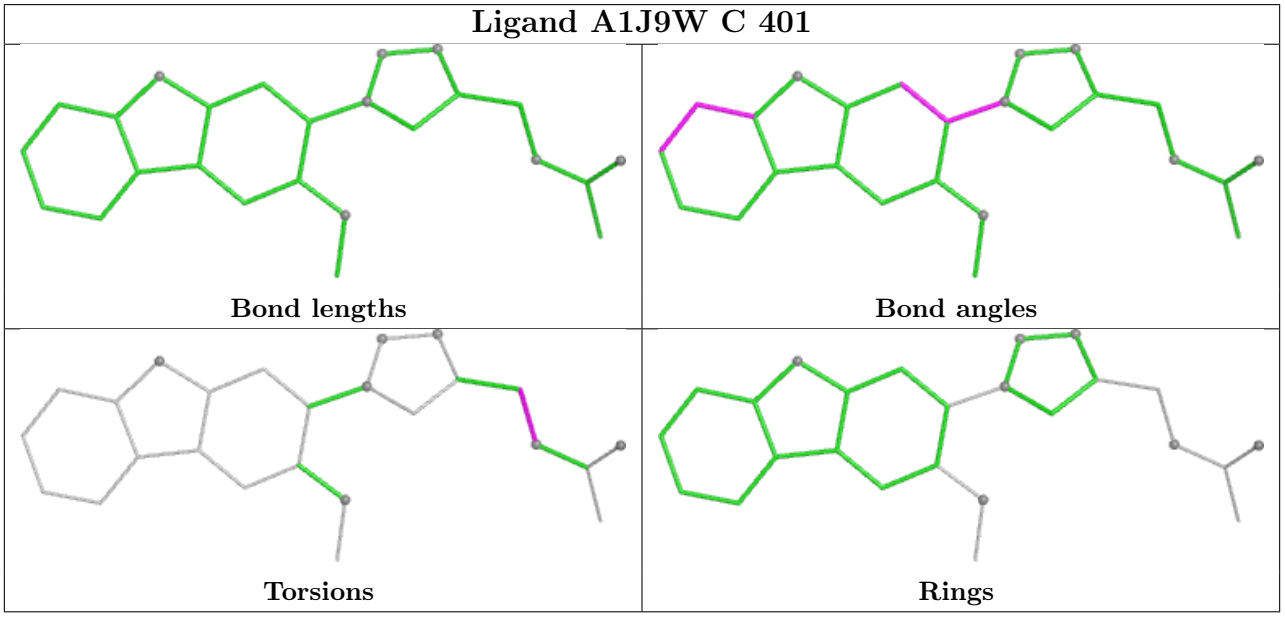
Mol	Chain	Res	Type	Atoms
2	G	401	A1J9W	C9-C10-N2-C11
2	A	401	A1J9W	C9-C10-N2-C11
2	B	401	A1J9W	C9-C10-N2-C11
2	C	401	A1J9W	C9-C10-N2-C11
2	D	401	A1J9W	C9-C10-N2-C11
2	E	401	A1J9W	C9-C10-N2-C11
2	F	401	A1J9W	C9-C10-N2-C11

There are no ring outliers.

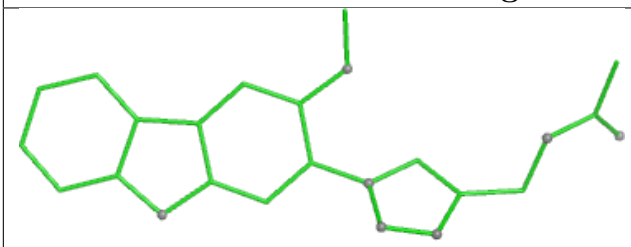
6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	A1J9W	1	0
2	G	401	A1J9W	1	0
2	A	401	A1J9W	1	0
2	B	401	A1J9W	1	0
2	E	401	A1J9W	1	0
2	D	401	A1J9W	1	0

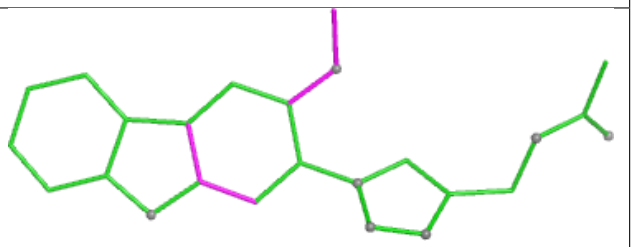
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



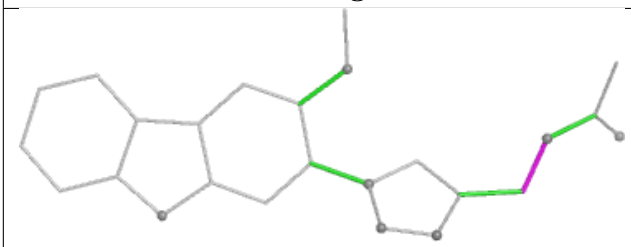
Ligand A1J9W G 401



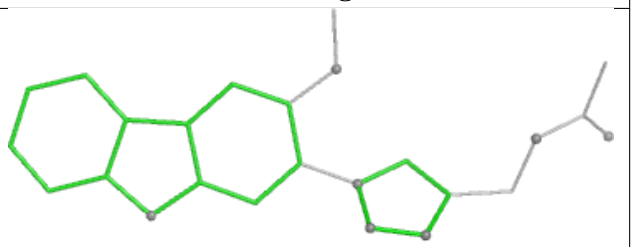
Bond lengths



Bond angles

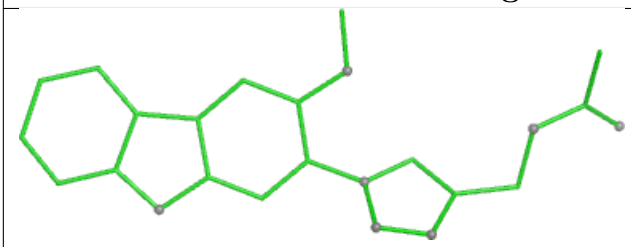


Torsions

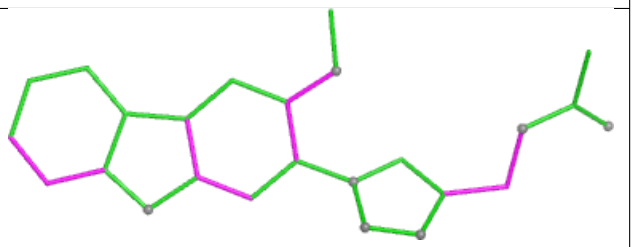


Rings

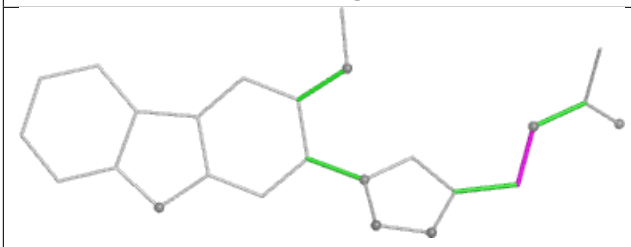
Ligand A1J9W A 401



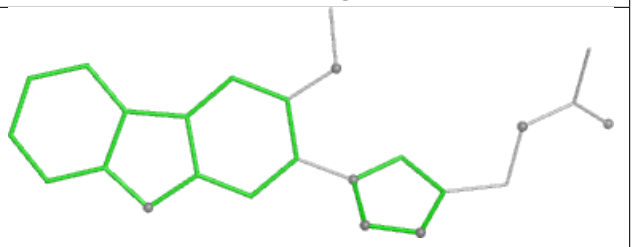
Bond lengths



Bond angles

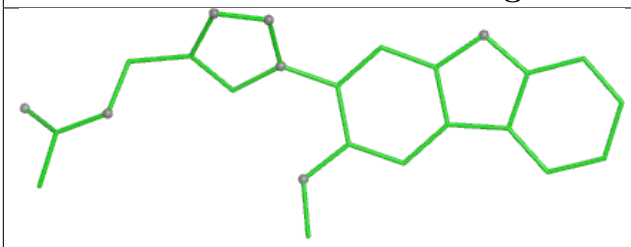


Torsions

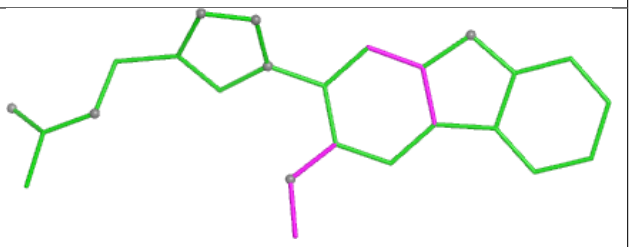


Rings

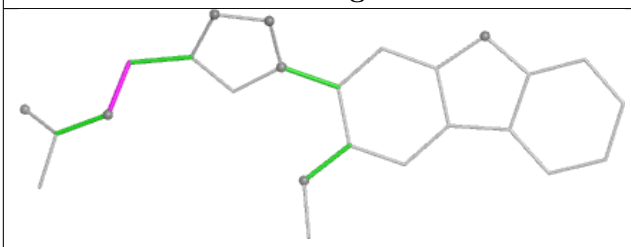
Ligand A1J9W F 401



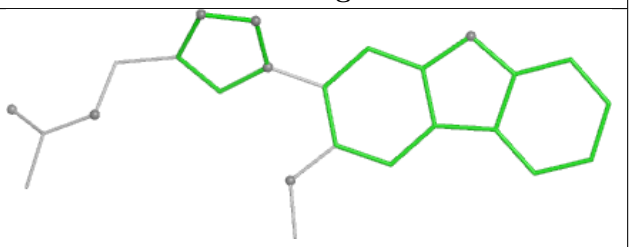
Bond lengths



Bond angles

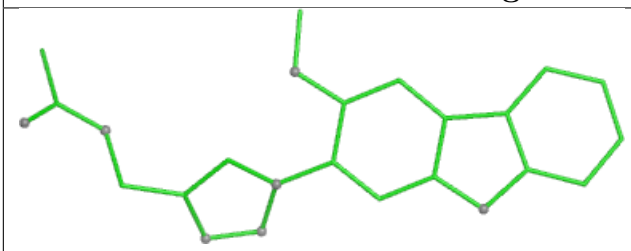


Torsions

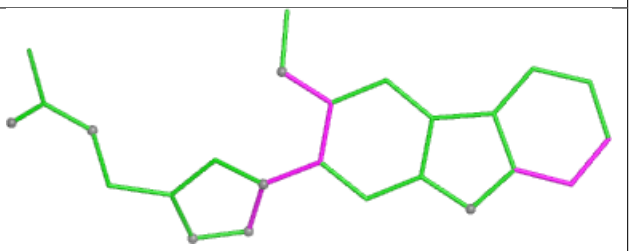


Rings

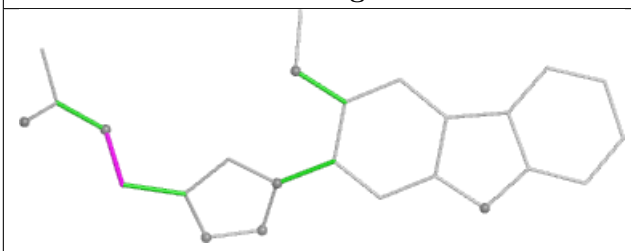
Ligand A1J9W B 401



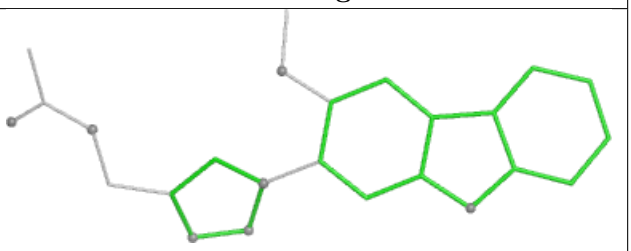
Bond lengths



Bond angles

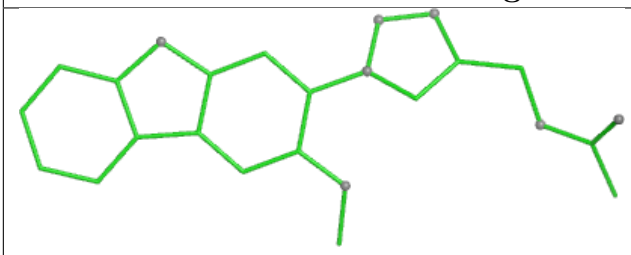


Torsions

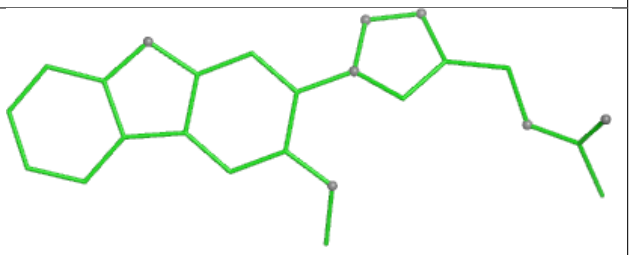


Rings

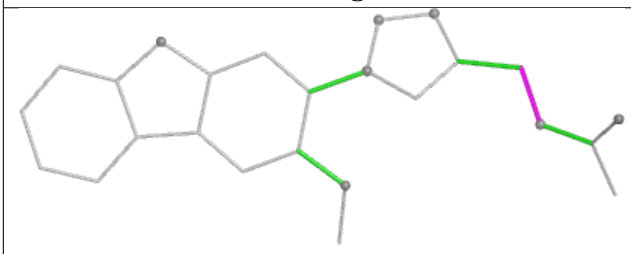
Ligand A1J9W E 401



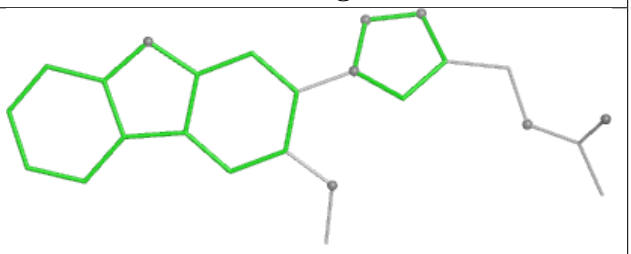
Bond lengths



Bond angles

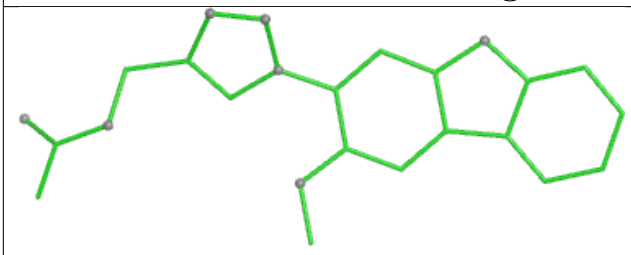


Torsions

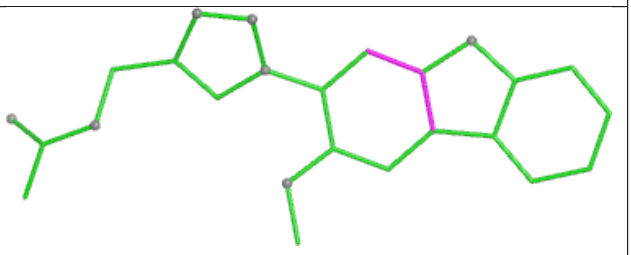


Rings

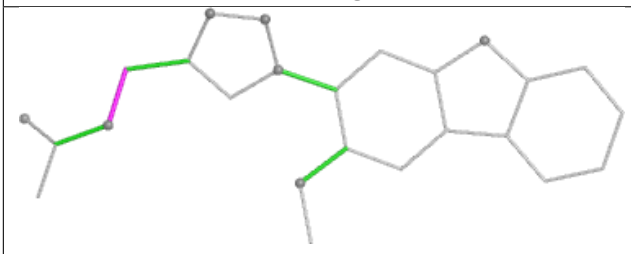
Ligand A1J9W D 401



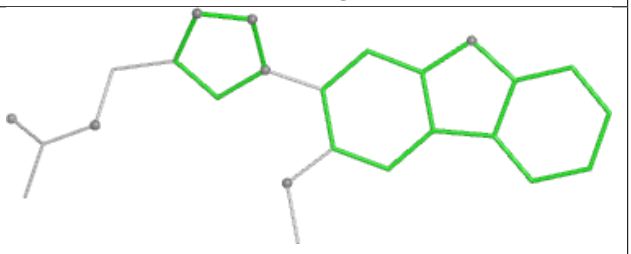
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	395/395 (100%)	0.12	15 (3%)	44	44	16, 26, 52, 76	0
1	B	395/395 (100%)	0.16	14 (3%)	47	48	15, 27, 52, 78	0
1	C	390/395 (98%)	0.44	15 (3%)	44	44	19, 34, 57, 81	0
1	D	387/395 (97%)	0.54	23 (5%)	28	28	19, 37, 60, 85	0
1	E	390/395 (98%)	1.12	77 (19%)	3	2	27, 48, 79, 102	0
1	F	386/395 (97%)	1.22	77 (19%)	3	2	25, 52, 88, 105	0
1	G	384/395 (97%)	1.43	96 (25%)	2	1	32, 55, 87, 104	0
1	H	386/395 (97%)	1.68	131 (33%)	1	0	35, 61, 91, 112	0
All	All	3113/3160 (98%)	0.83	448 (14%)	6	5	15, 42, 79, 112	0

All (448) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	358	PHE	6.0
1	G	366	HIS	6.0
1	E	358	PHE	5.0
1	E	30	PRO	4.8
1	H	30	PRO	4.8
1	E	145	LEU	4.7
1	H	37	ILE	4.7
1	H	360	GLU	4.5
1	H	34	LEU	4.5
1	E	37	ILE	4.5
1	H	248	ILE	4.4
1	H	35	ILE	4.4
1	G	358	PHE	4.3
1	F	144	GLY	4.3
1	H	361	GLU	4.2
1	E	365	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	20	ALA	4.2
1	G	145	LEU	4.2
1	E	293	ASP	4.2
1	G	353	PHE	4.2
1	H	28	VAL	4.1
1	E	390	ALA	4.0
1	G	343	VAL	4.0
1	F	23	ALA	4.0
1	C	392	LEU	3.9
1	E	22	LEU	3.9
1	G	346	TYR	3.9
1	H	366	HIS	3.9
1	F	22	LEU	3.9
1	E	190	GLY	3.9
1	E	34	LEU	3.9
1	F	176	VAL	3.8
1	E	28	VAL	3.8
1	H	246	SER	3.8
1	H	343	VAL	3.8
1	F	15	TYR	3.8
1	G	373	TYR	3.8
1	H	183	TYR	3.8
1	H	199	ALA	3.8
1	D	366	HIS	3.8
1	H	40	THR	3.8
1	F	341	VAL	3.8
1	H	17	VAL	3.8
1	G	63	ILE	3.7
1	H	364	ALA	3.7
1	H	377	ILE	3.7
1	E	356	VAL	3.7
1	F	17	VAL	3.7
1	G	337	ASN	3.7
1	F	349	PHE	3.7
1	E	391	ALA	3.7
1	H	346	TYR	3.7
1	G	349	PHE	3.6
1	G	21	LYS	3.6
1	G	341	VAL	3.6
1	E	15	TYR	3.5
1	H	63	ILE	3.5
1	E	389	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	24	GLU	3.5
1	D	356	VAL	3.5
1	H	22	LEU	3.4
1	D	355	ASP	3.4
1	A	395	HIS	3.4
1	B	396	HIS	3.4
1	H	223	SER	3.4
1	E	378	GLU	3.4
1	C	394	HIS	3.4
1	E	366	HIS	3.4
1	G	17	VAL	3.4
1	F	63	ILE	3.4
1	H	148	GLY	3.4
1	H	232	PHE	3.4
1	B	366	HIS	3.4
1	H	143	TYR	3.4
1	E	144	GLY	3.4
1	H	20	ALA	3.4
1	A	362	GLN	3.4
1	H	227	PHE	3.4
1	A	246	SER	3.3
1	G	47	VAL	3.3
1	G	342	SER	3.3
1	E	362	GLN	3.3
1	A	366	HIS	3.3
1	H	195	LEU	3.3
1	G	44	VAL	3.3
1	G	194	PRO	3.3
1	E	12	VAL	3.3
1	H	345	ALA	3.3
1	F	339	THR	3.2
1	F	28	VAL	3.2
1	G	34	LEU	3.2
1	H	200	LEU	3.2
1	H	259	LEU	3.2
1	H	363	ASP	3.2
1	H	342	SER	3.2
1	F	37	ILE	3.2
1	F	366	HIS	3.2
1	E	25	ALA	3.2
1	G	9	ASN	3.2
1	G	273	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	296	ALA	3.1
1	H	356	VAL	3.1
1	G	370	HIS	3.1
1	G	129	PRO	3.1
1	F	345	ALA	3.1
1	H	326	LEU	3.1
1	F	369	ARG	3.1
1	F	196	VAL	3.1
1	G	267	VAL	3.1
1	H	302	LEU	3.1
1	F	36	GLY	3.0
1	H	194	PRO	3.0
1	F	356	VAL	3.0
1	H	335	LEU	3.0
1	F	362	GLN	3.0
1	E	26	ARG	3.0
1	E	339	THR	3.0
1	G	327	ASP	3.0
1	G	365	VAL	3.0
1	H	47	VAL	3.0
1	E	377	ILE	3.0
1	G	252	ASP	3.0
1	H	33	PHE	3.0
1	H	358	PHE	3.0
1	H	234	VAL	3.0
1	A	360	GLU	3.0
1	E	173	GLU	3.0
1	F	35	ILE	3.0
1	F	51	ILE	3.0
1	H	193	TYR	3.0
1	E	353	PHE	3.0
1	H	182	VAL	2.9
1	B	221	GLY	2.9
1	A	358	PHE	2.9
1	G	190	GLY	2.9
1	F	293	ASP	2.9
1	F	346	TYR	2.9
1	F	246	SER	2.9
1	G	376	ASN	2.9
1	H	38	GLY	2.9
1	H	274	GLY	2.9
1	D	63	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	358	PHE	2.9
1	G	242	LYS	2.9
1	E	345	ALA	2.9
1	H	126	ALA	2.9
1	E	200	LEU	2.8
1	H	252	ASP	2.8
1	H	341	VAL	2.8
1	F	357	GLU	2.8
1	F	375	SER	2.8
1	E	33	PHE	2.8
1	H	288	LEU	2.8
1	G	158	VAL	2.8
1	G	356	VAL	2.8
1	G	146	ASN	2.8
1	E	344	ASP	2.8
1	F	363	ASP	2.8
1	F	25	ALA	2.8
1	G	361	GLU	2.8
1	B	356	VAL	2.8
1	G	291	ASN	2.8
1	A	354	ASP	2.8
1	G	40	THR	2.8
1	E	343	VAL	2.8
1	C	251	ALA	2.7
1	E	351	LYS	2.7
1	G	20	ALA	2.7
1	G	25	ALA	2.7
1	G	192	LYS	2.7
1	F	193	TYR	2.7
1	H	145	LEU	2.7
1	H	205	TYR	2.7
1	G	127	THR	2.7
1	H	146	ASN	2.7
1	H	379	ASN	2.7
1	D	359	ASP	2.7
1	F	359	ASP	2.7
1	E	274	GLY	2.7
1	H	262	GLY	2.7
1	G	351	LYS	2.7
1	F	33	PHE	2.7
1	G	126	ALA	2.7
1	H	352	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	299	THR	2.7
1	E	272	TYR	2.7
1	A	130	ASN	2.7
1	F	45	SER	2.7
1	G	375	SER	2.7
1	H	186	TRP	2.7
1	B	389	ALA	2.7
1	E	20	ALA	2.7
1	E	350	PHE	2.7
1	F	251	ALA	2.7
1	G	243	ALA	2.7
1	F	34	LEU	2.7
1	H	294	LEU	2.7
1	F	235	PRO	2.7
1	G	320	GLU	2.7
1	G	387	PRO	2.7
1	B	63	ILE	2.7
1	C	248	ILE	2.7
1	E	47	VAL	2.7
1	E	82	VAL	2.7
1	F	29	ASP	2.7
1	E	364	ALA	2.6
1	H	251	ALA	2.6
1	H	254	THR	2.6
1	H	303	PHE	2.6
1	E	375	SER	2.6
1	F	147	SER	2.6
1	G	183	TYR	2.6
1	E	242	LYS	2.6
1	G	234	VAL	2.6
1	F	148	GLY	2.6
1	G	186	TRP	2.6
1	H	19	MET	2.6
1	D	364	ALA	2.6
1	E	243	ALA	2.6
1	E	348	THR	2.6
1	F	145	LEU	2.6
1	H	235	PRO	2.6
1	A	355	ASP	2.6
1	G	32	LYS	2.6
1	E	39	GLN	2.6
1	H	297	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	367	GLU	2.6
1	H	253	GLU	2.6
1	H	239	MET	2.6
1	B	165	ASN	2.6
1	G	43	ALA	2.6
1	G	254	THR	2.6
1	E	387	PRO	2.6
1	H	244	LEU	2.6
1	H	372	PHE	2.6
1	H	247	ILE	2.6
1	H	365	VAL	2.6
1	D	370	HIS	2.6
1	B	130	ASN	2.6
1	E	31	ASN	2.6
1	D	218	LYS	2.6
1	H	32	LYS	2.6
1	B	129	PRO	2.6
1	H	29	ASP	2.6
1	H	349	PHE	2.5
1	H	263	TYR	2.5
1	G	189	THR	2.5
1	D	326	LEU	2.5
1	G	39	GLN	2.5
1	H	350	PHE	2.5
1	C	118	ILE	2.5
1	G	369	ARG	2.5
1	D	296	ALA	2.5
1	H	353	PHE	2.5
1	H	36	GLY	2.5
1	H	198	GLY	2.5
1	C	63	ILE	2.5
1	E	35	ILE	2.5
1	F	143	TYR	2.5
1	H	15	TYR	2.5
1	G	61	ASP	2.5
1	F	342	SER	2.5
1	H	224	LEU	2.5
1	H	144	GLY	2.5
1	E	381	VAL	2.4
1	H	196	VAL	2.4
1	H	273	VAL	2.4
1	E	66	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	223	SER	2.4
1	H	255	THR	2.4
1	H	348	THR	2.4
1	H	329	ALA	2.4
1	E	32	LYS	2.4
1	G	334	LEU	2.4
1	G	374	LEU	2.4
1	H	283	LEU	2.4
1	A	396	HIS	2.4
1	A	356	VAL	2.4
1	C	293	ASP	2.4
1	E	143	TYR	2.4
1	F	183	TYR	2.4
1	G	225	ALA	2.4
1	H	43	ALA	2.4
1	G	244	LEU	2.4
1	E	36	GLY	2.4
1	F	31	ASN	2.4
1	F	360	GLU	2.4
1	F	377	ILE	2.4
1	G	28	VAL	2.4
1	F	189	THR	2.4
1	G	26	ARG	2.4
1	H	14	LYS	2.4
1	H	189	THR	2.4
1	H	387	PRO	2.4
1	H	228	ALA	2.4
1	C	224	LEU	2.4
1	B	361	GLU	2.4
1	C	360	GLU	2.4
1	H	203	ASP	2.4
1	D	47	VAL	2.4
1	G	35	ILE	2.4
1	E	186	TRP	2.4
1	F	191	HIS	2.4
1	G	263	TYR	2.3
1	E	23	ALA	2.3
1	G	251	ALA	2.3
1	H	25	ALA	2.3
1	H	291	ASN	2.3
1	F	351	LYS	2.3
1	H	10	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	168	ILE	2.3
1	E	40	THR	2.3
1	G	2	THR	2.3
1	H	151	PRO	2.3
1	G	269	TYR	2.3
1	A	221	GLY	2.3
1	G	283	LEU	2.3
1	G	10	PHE	2.3
1	E	342	SER	2.3
1	B	173	GLU	2.3
1	F	264	GLU	2.3
1	F	340	GLU	2.3
1	F	40	THR	2.3
1	H	13	PRO	2.3
1	H	110	ALA	2.3
1	E	183	TYR	2.3
1	E	283	LEU	2.3
1	G	193	TYR	2.3
1	F	19	MET	2.3
1	F	350	PHE	2.3
1	G	173	GLU	2.3
1	E	276	ILE	2.3
1	G	46	PRO	2.3
1	H	152	THR	2.3
1	C	332	LYS	2.3
1	F	21	LYS	2.3
1	H	178	TYR	2.3
1	H	213	TRP	2.3
1	F	361	GLU	2.2
1	H	92	ILE	2.2
1	F	82	VAL	2.2
1	F	182	VAL	2.2
1	D	293	ASP	2.2
1	A	389	ALA	2.2
1	D	251	ALA	2.2
1	G	272	TYR	2.2
1	H	370	HIS	2.2
1	G	236	PHE	2.2
1	G	352	ARG	2.2
1	B	365	VAL	2.2
1	H	381	VAL	2.2
1	D	354	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	253	GLU	2.2
1	D	357	GLU	2.2
1	G	217	ALA	2.2
1	B	362	GLN	2.2
1	H	16	TYR	2.2
1	C	247	ILE	2.2
1	F	98	ILE	2.2
1	F	151	PRO	2.2
1	G	350	PHE	2.2
1	E	234	VAL	2.2
1	B	357	GLU	2.2
1	E	388	GLU	2.2
1	F	173	GLU	2.2
1	H	362	GLN	2.2
1	E	352	ARG	2.2
1	H	277	TYR	2.2
1	C	222	LYS	2.2
1	E	192	LYS	2.2
1	C	249	ASP	2.2
1	G	33	PHE	2.1
1	H	66	GLU	2.1
1	H	209	PHE	2.1
1	H	286	ILE	2.1
1	H	161	VAL	2.1
1	H	267	VAL	2.1
1	G	22	LEU	2.1
1	G	238	LYS	2.1
1	F	337	ASN	2.1
1	G	15	TYR	2.1
1	E	347	GLU	2.1
1	H	237	THR	2.1
1	D	295	GLN	2.1
1	E	191	HIS	2.1
1	F	365	VAL	2.1
1	G	12	VAL	2.1
1	G	191	HIS	2.1
1	G	196	VAL	2.1
1	G	385	HIS	2.1
1	H	26	ARG	2.1
1	H	260	ARG	2.1
1	E	147	SER	2.1
1	G	360	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	39	GLN	2.1
1	E	295	GLN	2.1
1	F	52	VAL	2.1
1	H	266	ALA	2.1
1	F	200	LEU	2.1
1	H	45	SER	2.1
1	H	375	SER	2.1
1	D	388	GLU	2.1
1	E	275	ASN	2.1
1	F	48	ASN	2.1
1	E	354	ASP	2.1
1	F	249	ASP	2.1
1	G	354	ASP	2.1
1	F	13	PRO	2.1
1	H	129	PRO	2.1
1	D	35	ILE	2.1
1	G	248	ILE	2.1
1	G	377	ILE	2.1
1	E	44	VAL	2.1
1	F	343	VAL	2.1
1	F	353	PHE	2.1
1	C	257	GLU	2.0
1	D	223	SER	2.1
1	E	199	ALA	2.1
1	F	43	ALA	2.1
1	F	364	ALA	2.1
1	G	296	ALA	2.1
1	H	89	ALA	2.1
1	H	386	ARG	2.0
1	E	38	GLY	2.0
1	G	143	TYR	2.0
1	G	144	GLY	2.0
1	F	371	ILE	2.0
1	D	360	GLU	2.0
1	D	378	GLU	2.0
1	E	273	VAL	2.0
1	E	361	GLU	2.0
1	G	59	ALA	2.0
1	E	376	ASN	2.0
1	G	230	LEU	2.0
1	H	39	GLN	2.0
1	H	334	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	293	ASP	2.0
1	E	324	ASP	2.0
1	F	226	ASP	2.0
1	H	344	ASP	2.0
1	H	111	CYS	2.0
1	E	21	LYS	2.0
1	A	129	PRO	2.0
1	F	348	THR	2.0
1	G	30	PRO	2.0
1	H	339	THR	2.0
1	H	272	TYR	2.0
1	H	305	TYR	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)

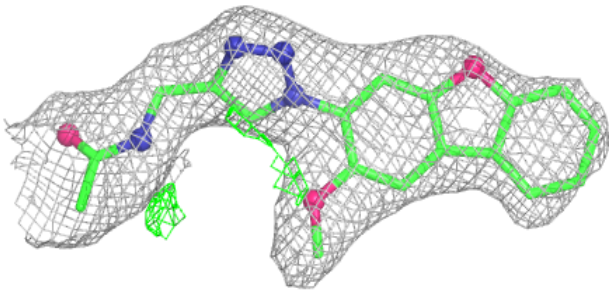
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

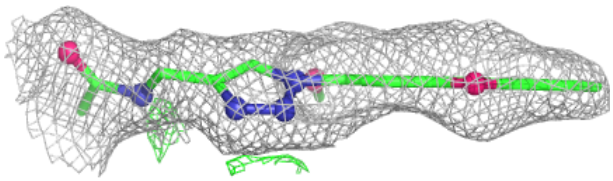
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1J9W	F	401	25/25	0.93	0.12	40,61,70,74	0
2	A1J9W	G	401	25/25	0.93	0.13	41,61,69,73	0
2	A1J9W	D	401	25/25	0.94	0.08	24,31,35,37	0
2	A1J9W	E	401	25/25	0.94	0.10	48,53,65,71	0
2	A1J9W	C	401	25/25	0.95	0.07	26,31,33,34	0
2	A1J9W	B	401	25/25	0.97	0.05	17,19,23,23	0
2	A1J9W	A	401	25/25	0.97	0.05	15,20,22,23	0

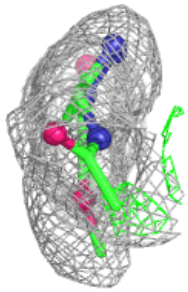
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1J9W F 401:

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

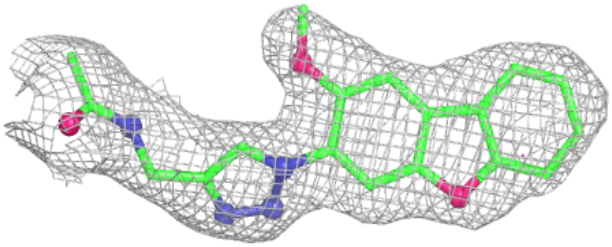


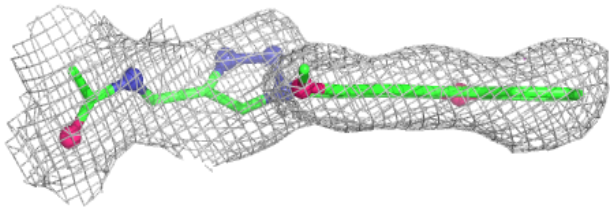


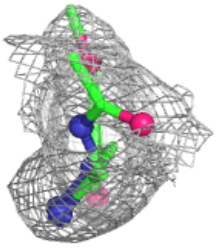


Electron density around A1J9W G 401:

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

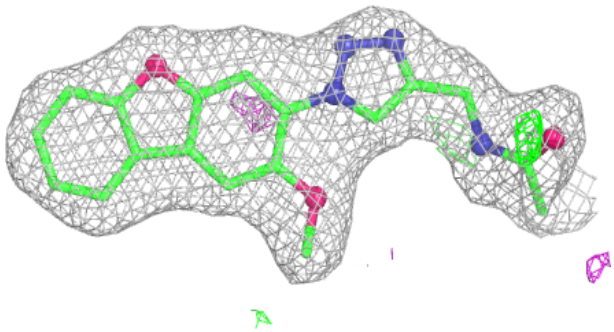


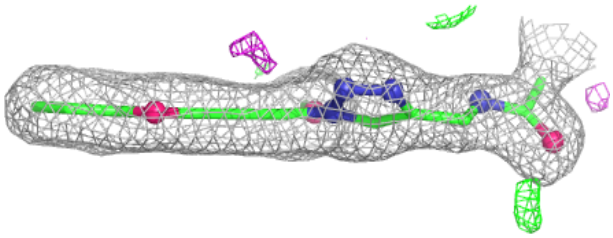


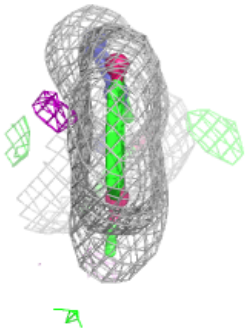


Electron density around A1J9W D 401:

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

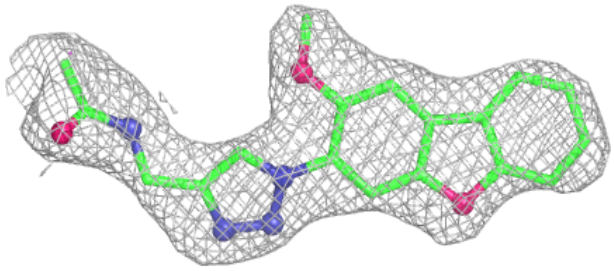


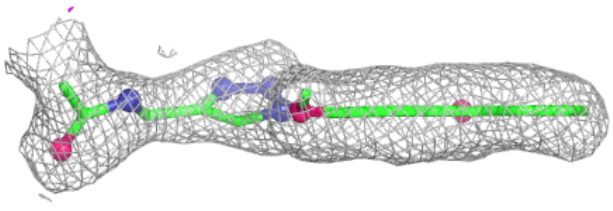


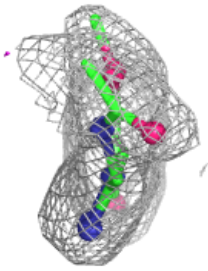


Electron density around A1J9W E 401:

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

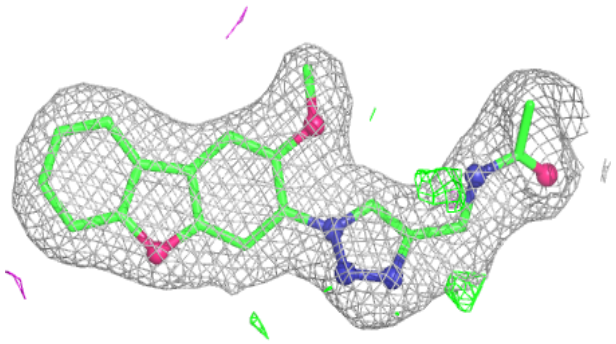


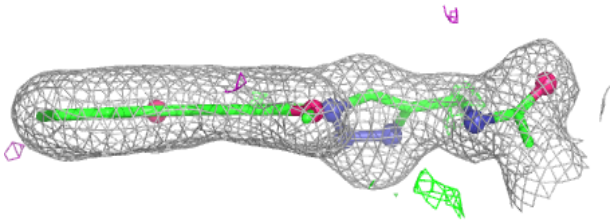


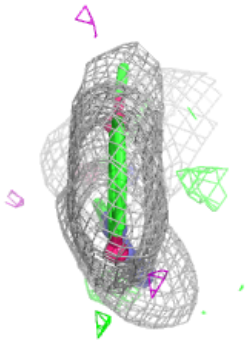


Electron density around A1J9W C 401:

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

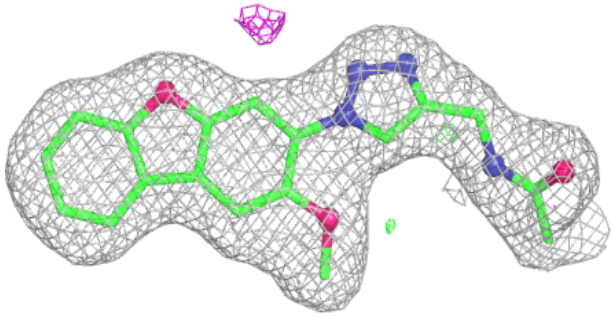


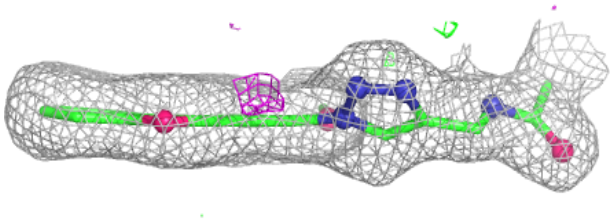


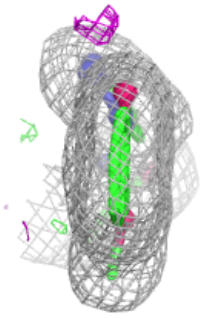


Electron density around A1J9W B 401:

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

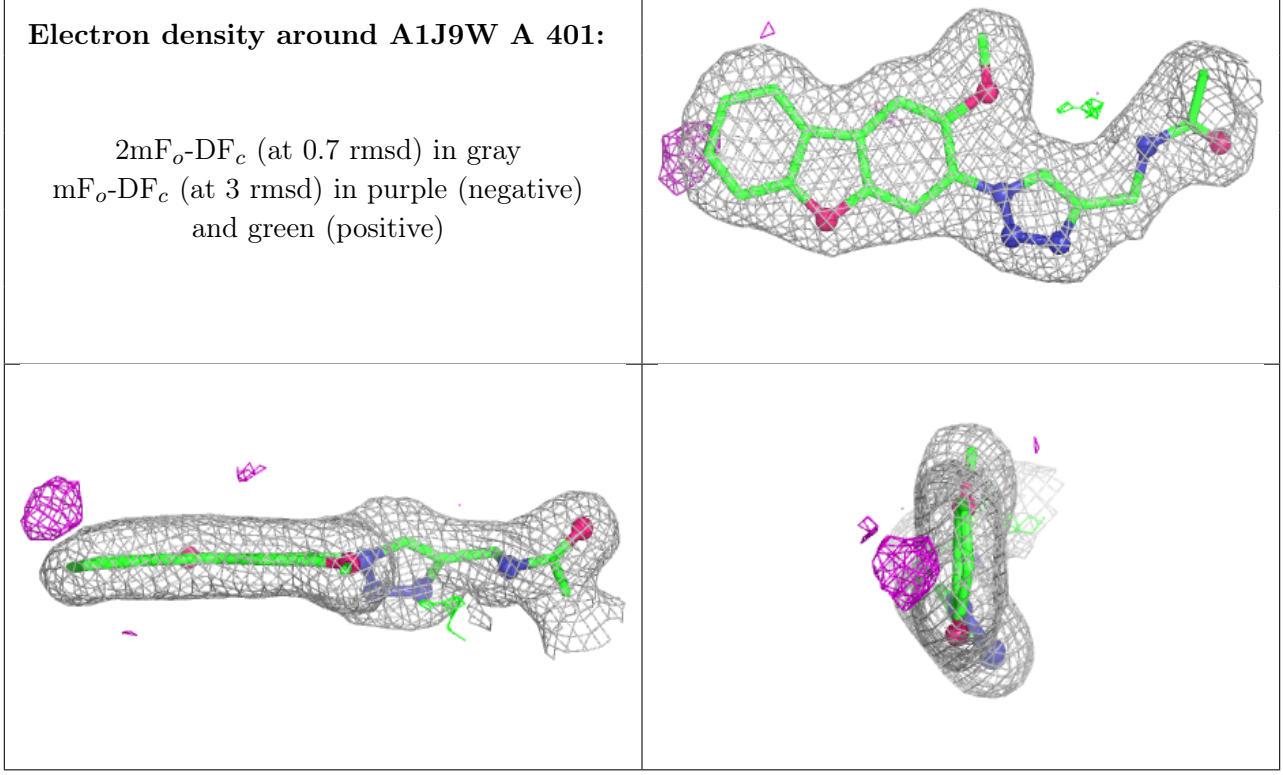






Electron density around A1J9W A 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.