



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:53 AM UTC

PDB ID : 2FA3 / pdb\_00002fa3  
Title : HMG-CoA synthase from Brassica juncea in complex with acetyl-CoA and acetyl-cys117.  
Authors : Pojer, F.; Ferrer, J.L.; Richard, S.B.; Noel, J.P.  
Deposited on : 2005-12-06  
Resolution : 2.52 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](mailto: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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

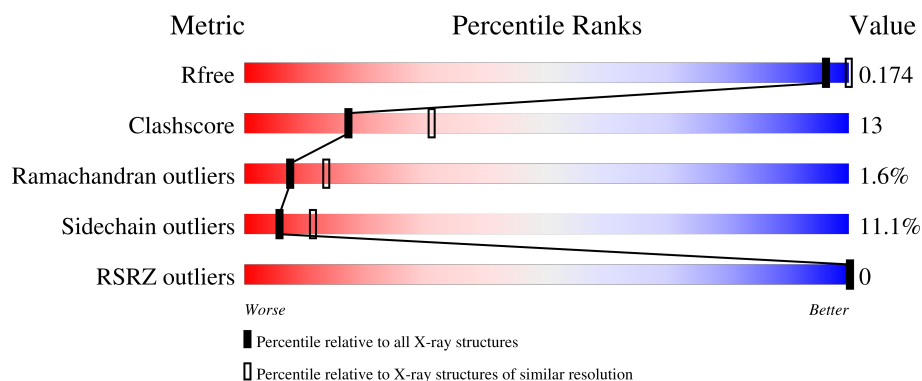
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	450	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3697 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.

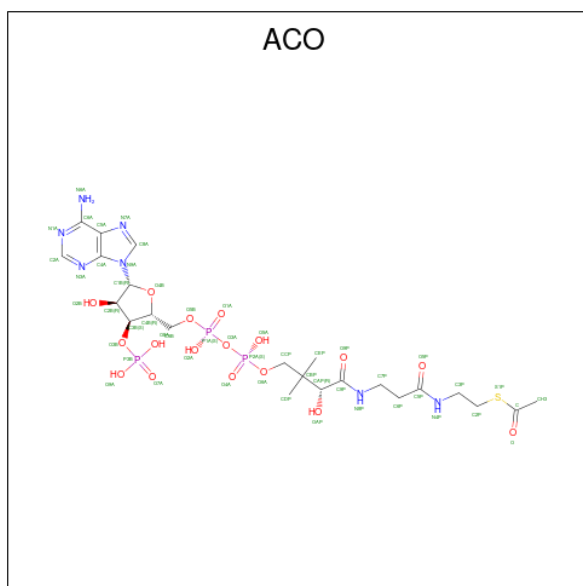
- Molecule 1 is a protein called HMG-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	450	3513	2239	575	676	23	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	SCY	CYS	modified residue	UNP Q9M6U3

- Molecule 2 is ACETYL COENZYME \*A (CCD ID: ACO) (formula:  $C_{23}H_{38}N_7O_{17}P_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P S		
2	A	1	51	23	7	17	3 1	0	0

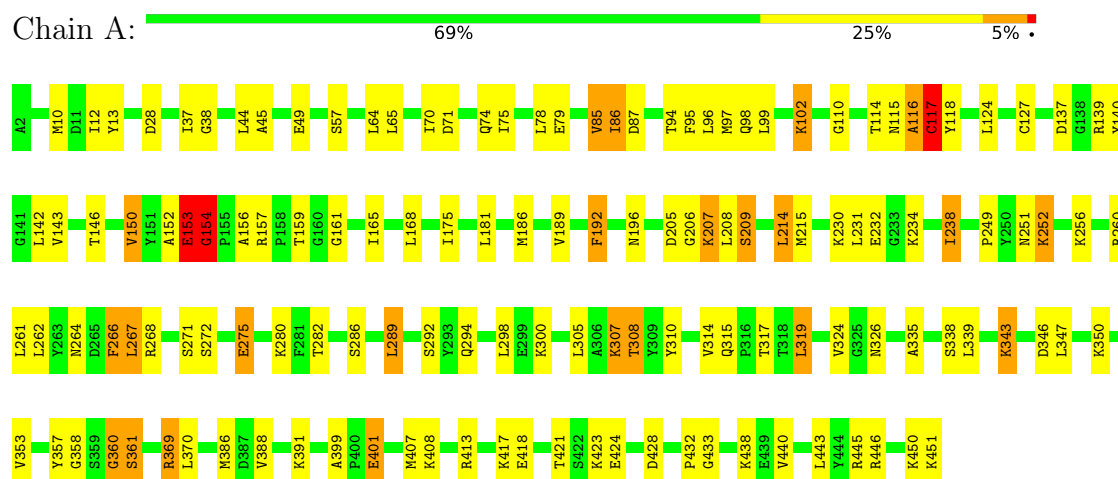
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	133	Total 133	O 133	0	0

### 3 Residue-property plots

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: HMG-CoA synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.60Å 61.60Å 411.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.52 50.00 – 2.52	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.52) 98.6 (50.00-2.52)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.176 , 0.282 0.182 , 0.174	Depositor DCC
$R_{free}$ test set	842 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.2	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3697	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: SCY, ACO

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	1.18	3/3579 (0.1%)	1.24	18/4833 (0.4%)

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	A	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	VAL	CA-CB	6.10	1.61	1.54
1	A	175	ILE	C-O	5.92	1.30	1.24
1	A	37	ILE	CA-CB	5.74	1.61	1.55

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	CYS	N-CA-C	7.85	119.84	111.28
1	A	154	GLY	CA-C-N	7.36	127.03	119.82
1	A	154	GLY	C-N-CA	7.36	127.03	119.82
1	A	231	LEU	N-CA-C	6.29	117.80	111.07
1	A	28	ASP	N-CA-C	-6.10	100.27	109.79
1	A	399	ALA	N-CA-C	-6.08	102.11	109.83
1	A	114	THR	N-CA-C	5.78	118.31	108.90
1	A	360	GLY	N-CA-C	-5.77	99.50	113.18
1	A	307	LYS	N-CA-C	5.62	118.17	111.71
1	A	118	TYR	CA-C-N	5.38	126.90	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	TYR	C-N-CA	5.38	126.90	120.13
1	A	251	ASN	N-CA-C	5.30	117.81	111.71
1	A	49	GLU	N-CA-C	-5.20	106.20	112.54
1	A	360	GLY	CA-C-N	5.15	131.38	121.54
1	A	360	GLY	C-N-CA	5.15	131.38	121.54
1	A	388	VAL	CA-C-N	5.04	125.53	119.94
1	A	388	VAL	C-N-CA	5.04	125.53	119.94
1	A	150	VAL	N-CA-C	5.03	115.90	108.45

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ALA	Mainchain,Peptide
1	A	117	SCY	Mainchain
1	A	360	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3513	0	3459	89	0
2	A	51	0	34	4	0
3	A	133	0	0	15	0
All	All	3697	0	3493	89	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 13.

All (89) 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:116:ALA:HB1	1:A:117:SCY:HE3	1.55	0.87
1:A:238:ILE:HD11	1:A:261:LEU:HB3	1.65	0.78
1:A:401:GLU:HB2	3:A:837:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LYS:NZ	1:A:207:LYS:HB2	1.98	0.78
1:A:369:ARG:HH11	1:A:369:ARG:HG3	1.49	0.77
1:A:117:SCY:OCD	2:A:796:ACO:HH31	1.88	0.73
1:A:408:LYS:HG2	3:A:909:HOH:O	1.89	0.72
1:A:369:ARG:HH11	1:A:369:ARG:CG	2.03	0.71
1:A:209:SER:HB2	2:A:796:ACO:H31	1.71	0.71
1:A:286:SER:HB2	3:A:925:HOH:O	1.91	0.71
1:A:205:ASP:O	1:A:209:SER:HB3	1.89	0.71
1:A:308:THR:HG23	3:A:928:HOH:O	1.91	0.70
1:A:238:ILE:HD11	1:A:261:LEU:CB	2.23	0.69
1:A:38:GLY:O	1:A:252:LYS:HD3	1.93	0.68
1:A:98:GLN:O	1:A:102:LYS:HE3	1.94	0.66
1:A:369:ARG:CG	1:A:369:ARG:NH1	2.58	0.65
1:A:300:LYS:HE3	3:A:902:HOH:O	1.96	0.65
1:A:137:ASP:OD1	1:A:139:ARG:HD3	1.96	0.65
1:A:266:PHE:O	1:A:268:ARG:N	2.31	0.63
1:A:86:ILE:CD1	1:A:446:ARG:HD2	2.28	0.63
1:A:432:PRO:HB3	1:A:451:LYS:NZ	2.14	0.63
1:A:238:ILE:CD1	1:A:261:LEU:HB3	2.28	0.62
1:A:153:GLU:HG2	1:A:154:GLY:H	1.65	0.61
1:A:196:ASN:HB3	3:A:915:HOH:O	1.99	0.61
1:A:407:MET:HA	1:A:407:MET:HE2	1.84	0.60
1:A:86:ILE:HD13	1:A:446:ARG:HD2	1.83	0.60
1:A:86:ILE:HD13	1:A:446:ARG:CD	2.32	0.59
1:A:157:ARG:HD2	3:A:926:HOH:O	2.02	0.58
1:A:192:PHE:CD2	1:A:192:PHE:C	2.81	0.58
1:A:443:LEU:HD12	1:A:445:ARG:NH1	2.18	0.58
1:A:207:LYS:HB2	1:A:207:LYS:HZ2	1.67	0.57
1:A:152:ALA:O	3:A:929:HOH:O	2.17	0.57
1:A:206:GLY:HA2	1:A:209:SER:OG	2.05	0.57
1:A:57:SER:OG	1:A:146:THR:HG21	2.05	0.56
1:A:433:GLY:H	1:A:451:LYS:HA	1.71	0.55
1:A:189:VAL:HG22	1:A:361:SER:HB2	1.87	0.55
1:A:308:THR:CG2	3:A:928:HOH:O	2.50	0.55
1:A:421:THR:O	1:A:423:LYS:NZ	2.39	0.55
1:A:153:GLU:CG	1:A:154:GLY:N	2.71	0.54
1:A:317:THR:HG22	1:A:339:LEU:HB2	1.90	0.54
1:A:153:GLU:HG2	1:A:154:GLY:N	2.23	0.53
1:A:208:LEU:O	1:A:209:SER:C	2.51	0.53
1:A:264:ASN:O	1:A:268:ARG:HG3	2.09	0.53
1:A:232:GLU:O	1:A:234:LYS:HE3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LEU:HA	3:A:868:HOH:O	2.09	0.52
1:A:249:PRO:HB3	2:A:796:ACO:HH32	1.91	0.52
1:A:86:ILE:HG13	1:A:87:ASP:N	2.25	0.51
1:A:252:LYS:HE3	2:A:796:ACO:O8A	2.10	0.51
1:A:192:PHE:C	1:A:192:PHE:HD2	2.19	0.51
1:A:275:GLU:HG3	3:A:888:HOH:O	2.12	0.50
1:A:38:GLY:O	1:A:252:LYS:CD	2.60	0.49
1:A:432:PRO:HB3	1:A:451:LYS:HZ2	1.77	0.49
1:A:386:MET:O	1:A:391:LYS:HE3	2.13	0.48
1:A:215:MET:CE	3:A:908:HOH:O	2.61	0.48
1:A:153:GLU:O	1:A:154:GLY:O	2.31	0.48
1:A:418:GLU:HA	1:A:440:VAL:O	2.14	0.48
1:A:417:LYS:NZ	3:A:913:HOH:O	2.47	0.47
1:A:215:MET:HE2	3:A:908:HOH:O	2.14	0.46
1:A:207:LYS:HB2	1:A:207:LYS:HZ3	1.79	0.46
1:A:424:GLU:HA	1:A:424:GLU:OE1	2.16	0.45
1:A:343:LYS:O	1:A:347:LEU:HG	2.15	0.45
1:A:450:LYS:CG	1:A:451:LYS:H	2.30	0.45
1:A:432:PRO:HB3	1:A:451:LYS:HZ3	1.80	0.45
1:A:78:LEU:HD12	1:A:79:GLU:N	2.32	0.44
1:A:161:GLY:HA3	1:A:326:ASN:O	2.17	0.43
1:A:215:MET:HE2	1:A:215:MET:HB3	1.86	0.43
1:A:110:GLY:HA2	3:A:857:HOH:O	2.17	0.43
1:A:214:LEU:HG	1:A:260:ARG:HD3	2.00	0.43
1:A:314:VAL:O	1:A:315:GLN:C	2.60	0.43
1:A:156:ALA:O	1:A:159:THR:OG1	2.36	0.43
1:A:335:ALA:O	1:A:338:SER:HB2	2.19	0.43
1:A:450:LYS:CG	1:A:451:LYS:N	2.82	0.42
1:A:115:ASN:O	1:A:116:ALA:C	2.62	0.42
1:A:140:TYR:HB3	1:A:168:LEU:HD11	2.01	0.42
1:A:346:ASP:O	1:A:350:LYS:HE2	2.19	0.42
1:A:124:LEU:HA	1:A:143:VAL:HG21	2.02	0.42
1:A:347:LEU:HB3	1:A:370:LEU:HD12	2.03	0.41
1:A:266:PHE:O	1:A:267:LEU:C	2.62	0.41
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.69	0.41
1:A:12:ILE:HG12	1:A:13:TYR:N	2.35	0.40
1:A:45:ALA:HB3	1:A:324:VAL:HG13	2.03	0.40
1:A:64:LEU:C	1:A:64:LEU:HD23	2.46	0.40
1:A:74:GLN:O	1:A:139:ARG:HB3	2.21	0.40
1:A:94:THR:O	1:A:97:MET:HB2	2.21	0.40
1:A:95:PHE:O	1:A:98:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:TYR:CD2	1:A:310:TYR:C	2.99	0.40
1:A:75:ILE:HD13	1:A:140:TYR:HB2	2.04	0.40
1:A:165:ILE:HD13	1:A:165:ILE:HG21	1.77	0.40
1:A:357:TYR:CG	1:A:358:GLY:N	2.90	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	447/450 (99%)	414 (93%)	26 (6%)	7 (2%)	7	13

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	GLU
1	A	267	LEU
1	A	361	SER
1	A	154	GLY
1	A	209	SER
1	A	266	PHE
1	A	272	SER

### 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	380/380 (100%)	338 (89%)	42 (11%)	6 11

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	44	LEU
1	A	65	LEU
1	A	70	ILE
1	A	71	ASP
1	A	85	VAL
1	A	86	ILE
1	A	96	LEU
1	A	99	LEU
1	A	102	LYS
1	A	142	LEU
1	A	150	VAL
1	A	153	GLU
1	A	181	LEU
1	A	186	MET
1	A	192	PHE
1	A	207	LYS
1	A	214	LEU
1	A	230	LYS
1	A	238	ILE
1	A	252	LYS
1	A	256	LYS
1	A	262	LEU
1	A	271	SER
1	A	275	GLU
1	A	280	LYS
1	A	282	THR
1	A	289	LEU
1	A	292	SER
1	A	294	GLN
1	A	298	LEU
1	A	305	LEU
1	A	307	LYS
1	A	308	THR
1	A	319	LEU
1	A	343	LYS
1	A	353	VAL
1	A	369	ARG

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Mol	Chain	Res	Type
1	A	401	GLU
1	A	413	ARG
1	A	428	ASP
1	A	438	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	115	ASN
1	A	304	GLN
1	A	342	ASN
1	A	344	HIS
1	A	381	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	SCY	A	117	1	7,8,9	1.56	2 (28%)	4,9,11	1.71	1 (25%)

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
1	SCY	A	117	1	-	3/5/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	SCY	CB-SG	-2.86	1.74	1.81
1	A	117	SCY	CA-N	-2.26	1.41	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	SCY	OCD-CD-SG	-2.37	113.08	122.65

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	117	SCY	OCD-CD-SG-CB
1	A	117	SCY	CE-CD-SG-CB
1	A	117	SCY	CA-CB-SG-CD

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	117	SCY	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	ACO	A	796	-	51,53,53	1.18	5 (9%)	73,79,79	2.32	27 (36%)

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	ACO	A	796	-	-	14/51/67/67	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	796	ACO	O-C	4.41	1.43	1.21
2	A	796	ACO	C5A-C6A	2.16	1.47	1.41
2	A	796	ACO	C8A-N9A	-2.11	1.34	1.37
2	A	796	ACO	P1A-O3A	2.05	1.61	1.59
2	A	796	ACO	P3B-O3B	2.03	1.63	1.59

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	796	ACO	C4A-N9A-C8A	6.04	112.08	105.74
2	A	796	ACO	N9A-C8A-N7A	-5.93	105.52	113.94
2	A	796	ACO	C3P-N4P-C5P	5.59	133.24	122.82
2	A	796	ACO	N3A-C2A-N1A	-5.56	120.17	128.58
2	A	796	ACO	C2P-C3P-N4P	-4.39	103.25	112.41
2	A	796	ACO	C5A-C4A-N3A	-3.96	121.27	126.72
2	A	796	ACO	C2A-N3A-C4A	3.80	121.10	111.83
2	A	796	ACO	N3A-C4A-N9A	3.78	133.59	127.17
2	A	796	ACO	C6P-C7P-N8P	-3.74	104.05	112.00
2	A	796	ACO	C7P-N8P-C9P	3.52	128.87	122.55
2	A	796	ACO	C5A-N7A-C8A	3.41	108.80	103.45
2	A	796	ACO	O3A-P2A-O4A	-3.30	100.77	110.70
2	A	796	ACO	O9A-P3B-O8A	2.98	118.96	107.80
2	A	796	ACO	C2P-S1P-C	2.94	115.56	101.42
2	A	796	ACO	O4B-C1B-N9A	-2.93	102.47	108.09
2	A	796	ACO	CEP-CBP-CCP	2.88	112.97	108.22
2	A	796	ACO	C7P-C6P-C5P	-2.83	107.69	112.39

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	796	ACO	O3A-P1A-O1A	-2.54	103.06	110.70
2	A	796	ACO	O2A-P1A-O1A	2.51	124.11	112.44
2	A	796	ACO	O6A-CCP-CBP	2.50	114.57	110.55
2	A	796	ACO	O8A-P3B-O3B	-2.49	96.14	105.85
2	A	796	ACO	O5A-P2A-O4A	2.43	123.73	112.44
2	A	796	ACO	C4A-N9A-C1B	-2.37	121.08	126.63
2	A	796	ACO	N6A-C6A-N1A	2.30	123.50	118.38
2	A	796	ACO	CAP-C9P-N8P	-2.29	112.13	116.48
2	A	796	ACO	O3B-C3B-C4B	-2.28	102.01	110.03
2	A	796	ACO	C5A-C6A-N6A	-2.06	118.20	123.29

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	796	ACO	P1A-O3A-P2A-O6A
2	A	796	ACO	CCP-O6A-P2A-O3A
2	A	796	ACO	CCP-O6A-P2A-O4A
2	A	796	ACO	CDP-CBP-CCP-O6A
2	A	796	ACO	CEP-CBP-CCP-O6A
2	A	796	ACO	CAP-CBP-CCP-O6A
2	A	796	ACO	O-C-S1P-C2P
2	A	796	ACO	CH3-C-S1P-C2P
2	A	796	ACO	C6P-C5P-N4P-C3P
2	A	796	ACO	O5P-C5P-N4P-C3P
2	A	796	ACO	CCP-O6A-P2A-O5A
2	A	796	ACO	P2A-O3A-P1A-O2A
2	A	796	ACO	P2A-O3A-P1A-O1A
2	A	796	ACO	C5P-C6P-C7P-N8P

There are no ring outliers.

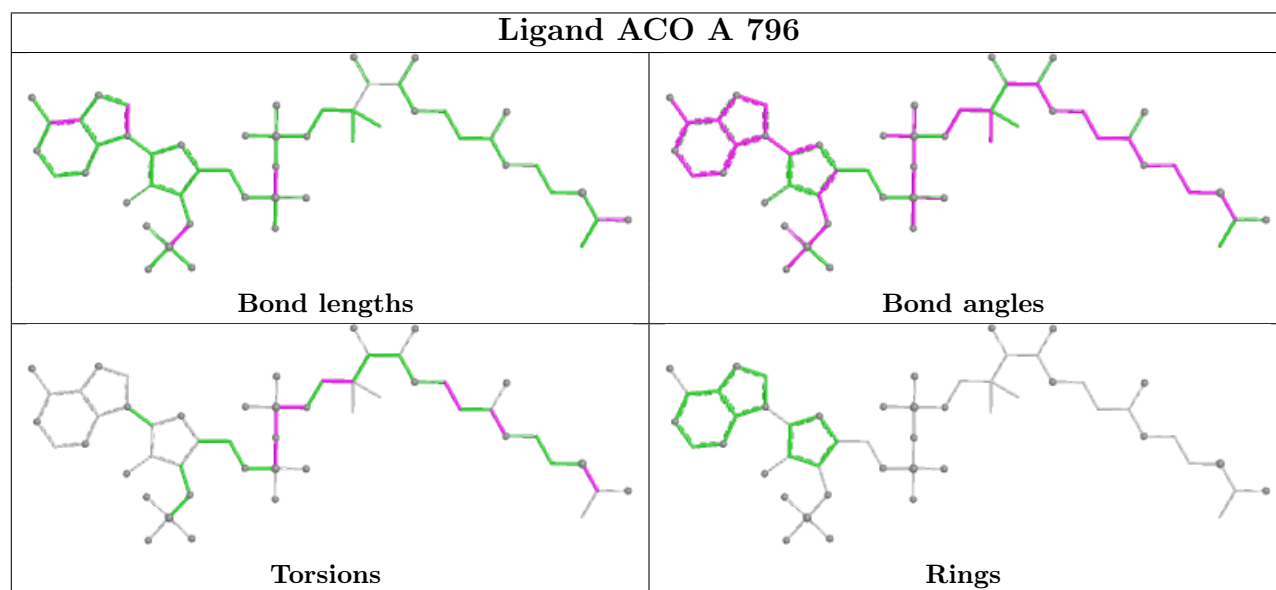
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	796	ACO	4	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 than 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.



## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	449/450 (99%)	-0.50	0 100 100	14, 29, 53, 63	0

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	SCY	A	117	9/10	0.95	0.09	23,24,36,45	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

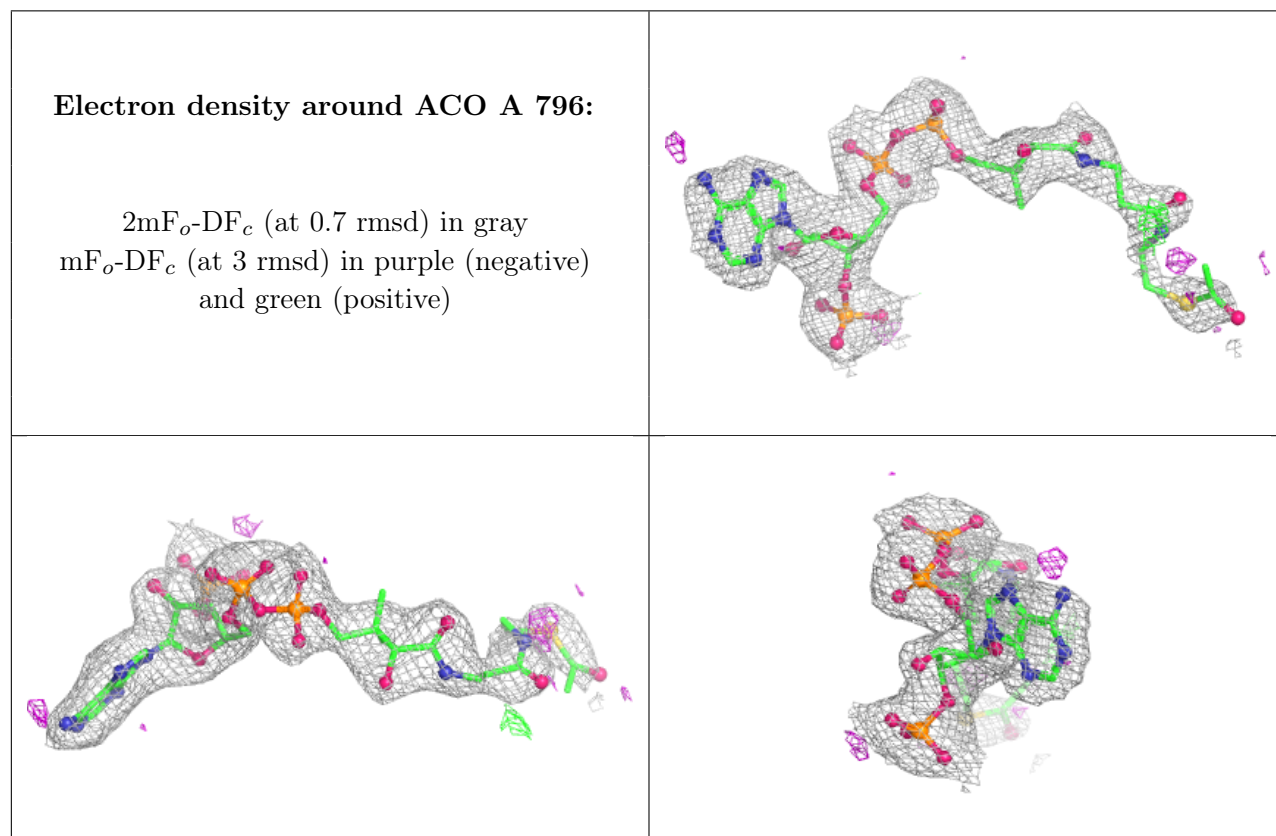
### 6.4 Ligands [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	ACO	A	796	51/51	0.94	0.09	38,46,62,65	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.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.