



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 07:39 PM BST

PDB ID : 4C49  
Title : Reactive loop cleaved human CBG in complex with cortisol  
Authors : Chan, W.L.; Zhou, A.; Read, R.J.  
Deposited on : 2013-09-02  
Resolution : 2.70 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

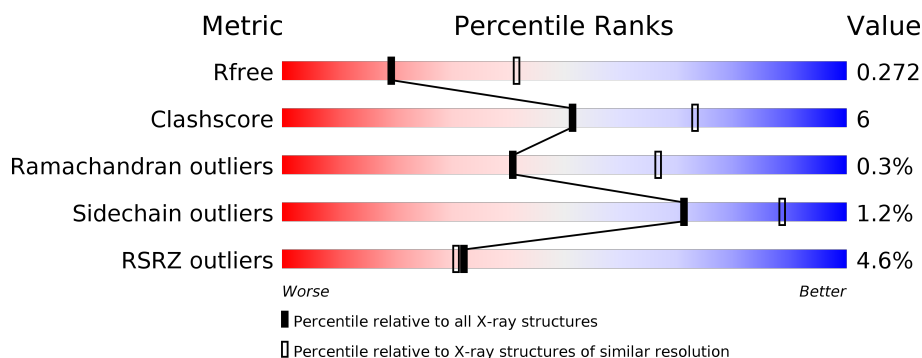
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	373	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>••</div> </div> </div>
1	B	373	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>••</div> </div> </div>
1	C	373	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>••</div> </div> </div>
1	D	373	<div> <div>11%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22751 atoms, of which 11319 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.

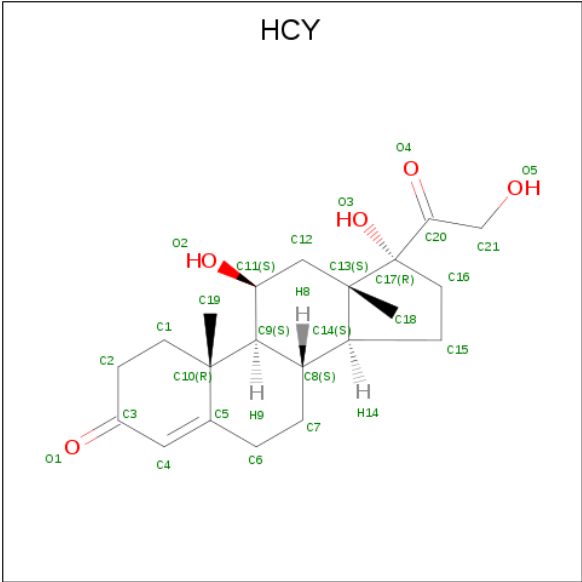
- Molecule 1 is a protein called CORTICOSTEROID-BINDING GLOBULIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	367	Total	C	H	N	O	S	0	0	0
			5652	1828	2804	469	537	14			
1	B	362	Total	C	H	N	O	S	1	0	0
			5621	1810	2804	467	526	14			
1	C	363	Total	C	H	N	O	S	14	0	0
			5684	1830	2834	471	535	14			
1	D	356	Total	C	H	N	O	S	1	0	0
			5532	1786	2757	461	514	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	ARG	THR	engineered mutation	UNP P08185
B	349	ARG	THR	engineered mutation	UNP P08185
C	349	ARG	THR	engineered mutation	UNP P08185
D	349	ARG	THR	engineered mutation	UNP P08185

- Molecule 2 is (11alpha,14beta)-11,17,21-trihydroxypregn-4-ene-3,20-dione (three-letter code: HCY) (formula: C<sub>21</sub>H<sub>30</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			56	21	30	5		
2	B	1	Total	C	H	O	0	0
			56	21	30	5		
2	C	1	Total	C	H	O	0	0
			56	21	30	5		
2	D	1	Total	C	H	O	0	0
			56	21	30	5		

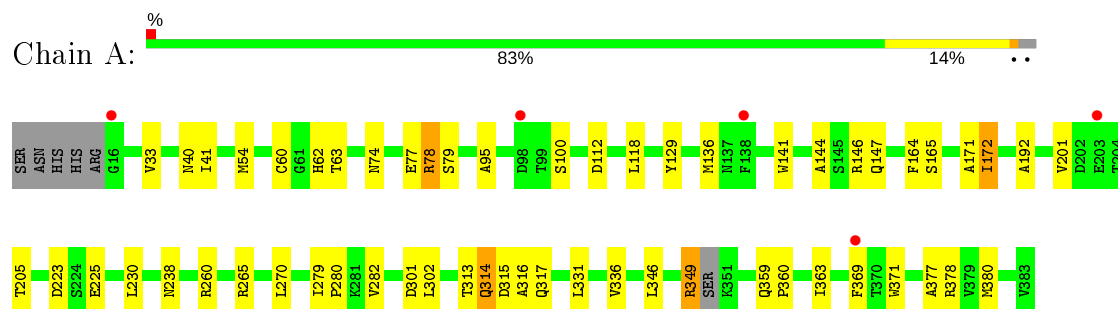
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	5	Total	O	0	0
			5	5		
3	C	13	Total	O	0	0
			13	13		
3	D	10	Total	O	0	0
			10	10		

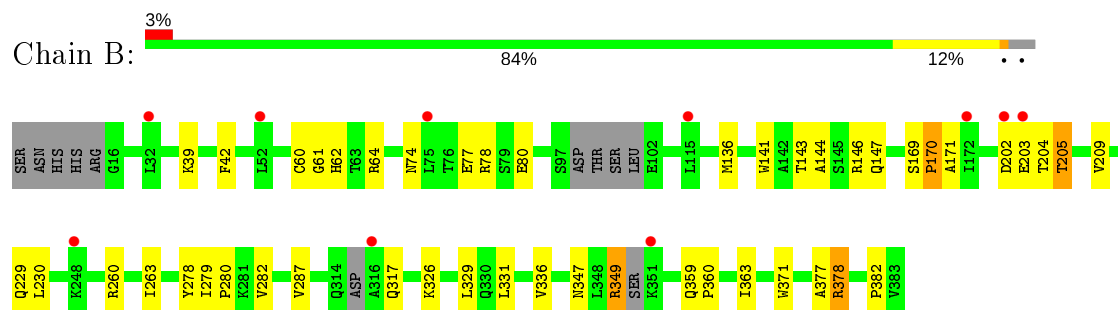
### 3 Residue-property plots

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.

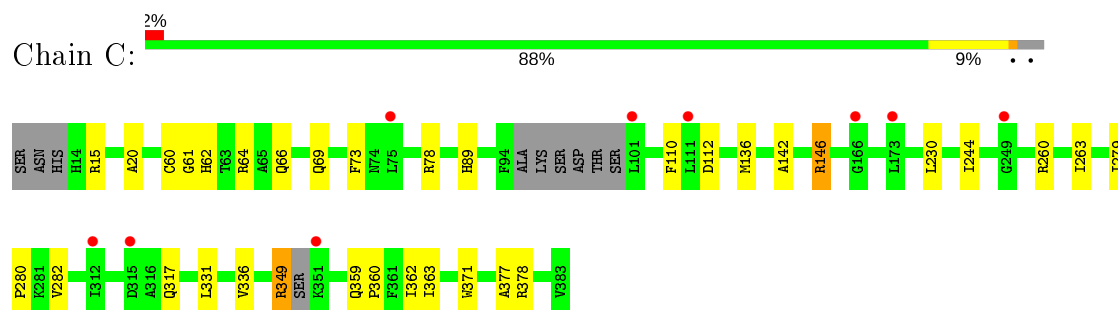
#### • Molecule 1: CORTICOSTEROID-BINDING GLOBULIN



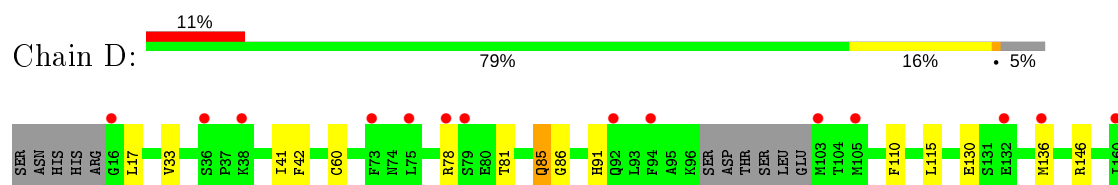
#### • Molecule 1: CORTICOSTEROID-BINDING GLOBULIN

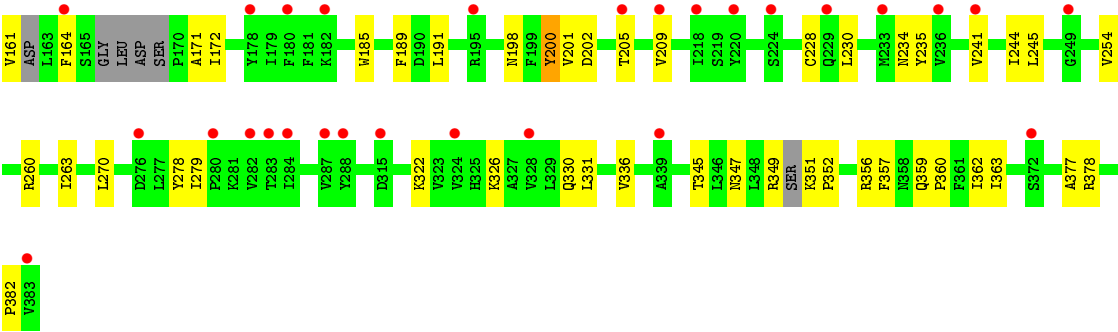


#### • Molecule 1: CORTICOSTEROID-BINDING GLOBULIN



#### • Molecule 1: CORTICOSTEROID-BINDING GLOBULIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.82Å 110.42Å 92.54Å 90.00° 102.52° 90.00°	Depositor
Resolution (Å)	69.92 – 2.70 69.92 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.9 (69.92-2.70) 94.6 (69.92-2.70)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1488)	Depositor
R, $R_{free}$	0.221 , 0.268 0.234 , 0.272	Depositor DCC
$R_{free}$ test set	1887 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.9	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	22751	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% 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: HCY

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	0.30	0/2907	3.91	5/3944 (0.1%)
1	B	0.30	0/2873	3.53	4/3890 (0.1%)
1	C	0.28	0/2908	3.51	4/3938 (0.1%)
1	D	0.29	0/2830	3.56	6/3831 (0.2%)
All	All	0.29	0/11518	3.63	19/15603 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	A	146	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	A	260	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	A	349	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	A	378	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	B	146	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	B	260	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	B	349	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	B	378	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	C	146	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	C	260	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	C	349	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	C	378	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	D	146	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	D	260	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	D	349	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	D	378	ARG	NH1-CZ-NH2	-108.55	0.00	119.40
1	D	201	VAL	N-CA-C	-5.67	95.70	111.00
1	D	200	TYR	N-CA-C	5.62	126.18	111.00



There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2848	2804	2801	33	0
1	B	2817	2804	2803	33	0
1	C	2850	2834	2834	23	1
1	D	2775	2757	2757	33	1
2	A	26	30	29	3	0
2	B	26	30	29	5	0
2	C	26	30	29	3	0
2	D	26	30	29	6	0
3	A	10	0	0	1	0
3	B	5	0	0	2	0
3	C	13	0	0	5	0
3	D	10	0	0	1	0
All	All	11432	11319	11311	127	1

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 6.

All (127) 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:C:112:ASP:OD1	3:C:2004:HOH:O	1.86	0.94
1:A:136:MET:SD	1:A:147:GLN:NE2	2.49	0.86
1:A:317:GLN:OE1	1:A:349:ARG:NH1	2.24	0.71
1:A:317:GLN:OE1	1:A:349:ARG:NH2	2.24	0.71
1:C:64:ARG:NH2	3:C:2002:HOH:O	2.16	0.70
1:B:263:ILE:HD11	2:B:1384:HCY:H191	1.73	0.70
1:C:60:CYS:SG	1:C:61:GLY:N	2.64	0.70
1:A:225:GLU:O	3:A:2005:HOH:O	2.09	0.69
1:B:170:PRO:O	1:B:347:ASN:ND2	2.26	0.69
2:D:1384:HCY:O5	3:D:2004:HOH:O	2.11	0.68
1:D:110:PHE:HB3	1:D:136:MET:SD	2.34	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:GLN:NE2	3:B:2002:HOH:O	2.28	0.65
1:B:74:ASN:HB3	1:B:77:GLU:HG2	1.79	0.63
1:C:60:CYS:SG	3:C:2002:HOH:O	2.55	0.63
1:A:201:VAL:HG13	1:A:205:THR:HB	1.80	0.62
1:B:64:ARG:NH1	1:B:80:GLU:OE1	2.35	0.59
1:A:95:ALA:O	1:A:100:SER:OG	2.21	0.59
1:C:263:ILE:CD1	2:C:1384:HCY:H191	2.32	0.59
2:D:1384:HCY:H193	2:D:1384:HCY:O2	2.03	0.58
1:C:263:ILE:HD11	2:C:1384:HCY:H191	1.86	0.58
1:B:278:TYR:OH	3:B:2003:HOH:O	2.18	0.57
1:D:263:ILE:CD1	2:D:1384:HCY:H191	2.36	0.56
1:A:371:TRP:HB3	2:A:1384:HCY:H7C1	1.87	0.55
1:B:263:ILE:CD1	2:B:1384:HCY:H191	2.35	0.55
1:D:81:THR:O	1:D:85:GLN:HG3	2.07	0.54
1:C:15:ARG:HD3	1:C:371:TRP:CD2	2.43	0.54
1:B:39:LYS:O	1:B:378:ARG:NH2	2.42	0.53
1:D:351:LYS:N	1:D:352:PRO:CD	2.72	0.52
1:D:33:VAL:HA	1:D:41:ILE:CD1	2.39	0.52
1:C:146:ARG:NH1	3:C:2007:HOH:O	2.42	0.51
1:C:146:ARG:NH2	3:C:2007:HOH:O	2.42	0.51
1:A:201:VAL:HG13	1:A:205:THR:O	2.11	0.51
1:C:69:GLN:NE2	1:D:189:PHE:O	2.42	0.51
1:B:141:TRP:HA	1:B:144:ALA:HB3	1.92	0.51
1:D:263:ILE:HD11	2:D:1384:HCY:H191	1.92	0.50
2:C:1384:HCY:O2	2:C:1384:HCY:H193	2.11	0.49
1:C:142:ALA:O	1:C:146:ARG:HG3	2.12	0.49
1:A:118:LEU:HD21	1:A:314:GLN:HB3	1.94	0.49
1:D:115:LEU:HD11	1:D:172:ILE:HD13	1.94	0.49
1:A:282:VAL:HB	1:A:331:LEU:HD12	1.94	0.49
1:B:363:ILE:HB	1:B:377:ALA:HB3	1.94	0.49
1:D:171:ALA:HB2	1:D:345:THR:HB	1.94	0.48
1:D:331:LEU:CD2	1:D:336:VAL:HG22	2.43	0.48
1:D:279:ILE:HG22	1:D:357:PHE:CD1	2.49	0.48
1:B:60:CYS:SG	1:B:61:GLY:N	2.87	0.48
2:A:1384:HCY:H193	2:A:1384:HCY:O2	2.13	0.48
2:B:1384:HCY:O2	2:B:1384:HCY:H193	2.14	0.47
1:B:141:TRP:CD1	1:B:169:SER:HB3	2.50	0.47
1:D:245:LEU:HB2	1:D:357:PHE:CE2	2.49	0.47
1:B:359:GLN:HB2	1:B:360:PRO:HD2	1.97	0.47
1:D:209:VAL:HG21	1:D:382:PRO:HB2	1.97	0.47
1:B:209:VAL:HG21	1:B:382:PRO:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:LYS:O	1:B:378:ARG:NH1	2.42	0.47
1:B:287:VAL:CG1	1:B:326:LYS:HD2	2.45	0.47
1:D:172:ILE:HG13	1:D:347:ASN:HA	1.96	0.47
1:C:317:GLN:OE1	1:C:349:ARG:NH2	2.48	0.46
1:C:317:GLN:OE1	1:C:349:ARG:NH1	2.48	0.46
1:A:192:ALA:HB3	1:B:62:HIS:CE1	2.51	0.46
1:D:228:CYS:HB3	1:D:254:VAL:HG21	1.98	0.46
1:D:42:PHE:HD1	1:D:377:ALA:HB2	1.81	0.46
1:A:201:VAL:CG1	1:A:205:THR:O	2.64	0.46
1:D:351:LYS:N	1:D:352:PRO:HD2	2.30	0.46
1:A:201:VAL:HG11	1:A:205:THR:HG22	1.98	0.46
1:A:62:HIS:ND1	1:A:301:ASP:OD2	2.48	0.46
1:B:203:GLU:HG3	1:B:204:THR:HG23	1.98	0.46
1:D:17:LEU:HD13	1:D:86:GLY:HA3	1.98	0.46
1:A:164:PHE:O	1:A:165:SER:OG	2.23	0.45
1:A:223:ASP:OD2	1:A:265:ARG:NH2	2.49	0.45
1:B:263:ILE:HD12	2:B:1384:HCY:H8	1.98	0.45
1:A:118:LEU:HG	1:A:313:THR:HA	1.98	0.45
1:A:33:VAL:HA	1:A:41:ILE:CD1	2.46	0.45
1:B:42:PHE:HD1	1:B:377:ALA:HB2	1.81	0.45
2:D:1384:HCY:H211	2:D:1384:HCY:H121	1.98	0.45
1:D:363:ILE:HB	1:D:377:ALA:HB3	1.98	0.45
1:D:91:HIS:CE1	1:D:130:GLU:HB3	2.52	0.45
1:D:161:VAL:O	1:D:326:LYS:NZ	2.40	0.45
1:A:363:ILE:HB	1:A:377:ALA:HB3	1.98	0.44
1:A:54:MET:HG3	1:A:129:TYR:CD1	2.53	0.44
1:C:363:ILE:HB	1:C:377:ALA:HB3	2.00	0.44
1:B:317:GLN:OE1	1:B:349:ARG:NH2	2.51	0.44
1:B:317:GLN:OE1	1:B:349:ARG:NH1	2.51	0.44
1:C:279:ILE:HG23	1:C:280:PRO:HD2	1.98	0.44
1:C:62:HIS:O	1:C:66:GLN:HB2	2.17	0.44
1:B:287:VAL:HG13	1:B:326:LYS:NZ	2.31	0.44
1:B:171:ALA:HA	1:B:347:ASN:ND2	2.33	0.44
1:C:359:GLN:HB2	1:C:360:PRO:HD2	1.97	0.44
1:C:331:LEU:HD23	1:C:336:VAL:HG22	1.98	0.44
1:A:112:ASP:CB	1:A:172:ILE:HG22	2.48	0.44
1:B:202:ASP:HB2	1:B:205:THR:OG1	2.18	0.44
1:A:40:ASN:OD1	1:A:380:MET:N	2.46	0.43
1:A:238:ASN:OD1	1:A:369:PHE:CD1	2.72	0.43
1:B:371:TRP:CE3	2:B:1384:HCY:H1C2	2.54	0.43
1:A:359:GLN:HB2	1:A:360:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1384:HCY:H211	2:A:1384:HCY:H121	2.00	0.43
1:B:42:PHE:CZ	1:B:329:LEU:HB2	2.54	0.43
1:D:235:TYR:OH	1:D:336:VAL:HG21	2.19	0.42
1:D:198:ASN:HB3	1:D:200:TYR:CE1	2.54	0.42
1:D:331:LEU:HD23	1:D:336:VAL:HG22	2.01	0.42
1:D:359:GLN:HB2	1:D:360:PRO:HD2	2.00	0.42
1:A:279:ILE:HG23	1:A:280:PRO:HD2	2.02	0.42
1:A:230:LEU:HD12	1:A:270:LEU:HD21	2.00	0.42
1:B:143:THR:O	1:B:147:GLN:HG3	2.20	0.42
1:D:185:TRP:HZ3	1:D:241:VAL:HG11	1.84	0.42
1:C:20:ALA:HB3	1:C:73:PHE:CE1	2.54	0.42
1:D:164:PHE:HE2	1:D:345:THR:CG2	2.33	0.42
1:D:244:ILE:HB	1:D:362:ILE:HB	2.01	0.42
1:A:331:LEU:CD2	1:A:336:VAL:HG22	2.49	0.42
1:B:279:ILE:HG23	1:B:280:PRO:HD2	2.01	0.42
1:C:282:VAL:HB	1:C:331:LEU:HD12	2.00	0.42
1:A:74:ASN:OD1	1:A:77:GLU:HG2	2.20	0.42
1:B:136:MET:HE3	1:B:144:ALA:CB	2.50	0.42
1:D:230:LEU:HD12	1:D:270:LEU:HD21	2.01	0.42
1:A:314:GLN:CG	1:A:315:ASP:N	2.83	0.41
1:A:171:ALA:HB1	1:A:346:LEU:O	2.19	0.41
1:C:110:PHE:CD1	1:C:136:MET:SD	3.14	0.41
2:D:1384:HCY:C12	2:D:1384:HCY:H211	2.51	0.41
1:D:245:LEU:HD11	1:D:359:GLN:CG	2.50	0.41
1:D:278:TYR:HB2	1:D:356:ARG:HA	2.01	0.41
1:B:282:VAL:HB	1:B:331:LEU:HD12	2.02	0.41
1:C:69:GLN:HG3	1:D:191:LEU:HD12	2.01	0.41
1:A:63:THR:CG2	1:A:302:LEU:HD23	2.51	0.41
1:A:141:TRP:HA	1:A:144:ALA:HB3	2.02	0.41
1:B:136:MET:HE3	1:B:144:ALA:HB1	2.02	0.41
1:A:74:ASN:HB3	1:A:77:GLU:HG2	2.03	0.41
1:B:331:LEU:HD23	1:B:336:VAL:HG22	2.02	0.40
1:C:244:ILE:HB	1:C:362:ILE:HB	2.04	0.40
1:D:322:LYS:N	1:D:345:THR:OG1	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:CYS:HG	1:D:60:CYS:SG[2_546]	1.28	0.32

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	363/373 (97%)	358 (99%)	4 (1%)	1 (0%)	41	66
1	B	354/373 (95%)	350 (99%)	3 (1%)	1 (0%)	41	66
1	C	357/373 (96%)	353 (99%)	4 (1%)	0	100	100
1	D	346/373 (93%)	339 (98%)	5 (1%)	2 (1%)	25	50
All	All	1420/1492 (95%)	1400 (99%)	16 (1%)	4 (0%)	41	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	202	ASP
1	A	316	ALA
1	D	205	THR
1	B	170	PRO

### 5.3.2 Protein sidechains ⓘ

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	313/328 (95%)	308 (98%)	5 (2%)	62	85
1	B	311/328 (95%)	308 (99%)	3 (1%)	76	91
1	C	318/328 (97%)	315 (99%)	3 (1%)	78	92
1	D	304/328 (93%)	300 (99%)	4 (1%)	69	87
All	All	1246/1312 (95%)	1231 (99%)	15 (1%)	71	88

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	CYS
1	A	78	ARG
1	A	79	SER
1	A	172	ILE
1	A	314	GLN
1	B	78	ARG
1	B	205	THR
1	B	230	LEU
1	C	78	ARG
1	C	89	HIS
1	C	230	LEU
1	D	78	ARG
1	D	85	GLN
1	D	234	ASN
1	D	330	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	147	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 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	HCY	A	1384	-	29,29,29	3.94	13 (44%)	48,48,48	5.32	21 (43%)
2	HCY	C	1384	-	29,29,29	3.90	13 (44%)	48,48,48	5.29	22 (45%)
2	HCY	B	1384	-	29,29,29	3.91	13 (44%)	48,48,48	5.24	27 (56%)
2	HCY	D	1384	-	29,29,29	3.90	13 (44%)	48,48,48	5.30	21 (43%)

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	HCY	A	1384	-	-	4/8/73/73	0/4/4/4
2	HCY	C	1384	-	-	5/8/73/73	0/4/4/4
2	HCY	B	1384	-	-	7/8/73/73	0/4/4/4
2	HCY	D	1384	-	-	7/8/73/73	0/4/4/4

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1384	HCY	C9-C11	9.72	1.70	1.53
2	C	1384	HCY	C9-C11	9.62	1.70	1.53
2	D	1384	HCY	C9-C11	9.39	1.69	1.53
2	A	1384	HCY	C9-C11	9.31	1.69	1.53
2	D	1384	HCY	O2-C11	-8.82	1.24	1.43
2	C	1384	HCY	O2-C11	-8.81	1.24	1.43
2	A	1384	HCY	O2-C11	-8.79	1.24	1.43
2	B	1384	HCY	O2-C11	-8.61	1.25	1.43
2	A	1384	HCY	C12-C11	8.16	1.65	1.53
2	B	1384	HCY	C12-C11	8.11	1.65	1.53
2	D	1384	HCY	C12-C11	7.85	1.65	1.53
2	C	1384	HCY	C12-C11	7.83	1.65	1.53
2	A	1384	HCY	C10-C9	-7.49	1.41	1.56
2	D	1384	HCY	C10-C9	-7.19	1.42	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1384	HCY	C10-C9	-7.11	1.42	1.56
2	B	1384	HCY	C10-C9	-6.97	1.43	1.56
2	A	1384	HCY	C16-C17	5.67	1.63	1.54
2	C	1384	HCY	C16-C17	5.62	1.63	1.54
2	D	1384	HCY	C16-C17	5.58	1.63	1.54
2	B	1384	HCY	C16-C17	5.57	1.63	1.54
2	D	1384	HCY	C13-C14	-5.37	1.44	1.54
2	A	1384	HCY	C17-C20	-5.36	1.44	1.53
2	B	1384	HCY	C13-C14	-5.34	1.44	1.54
2	D	1384	HCY	C6-C5	5.25	1.59	1.50
2	A	1384	HCY	C13-C14	-5.23	1.45	1.54
2	A	1384	HCY	C6-C5	5.21	1.59	1.50
2	B	1384	HCY	C6-C5	5.19	1.59	1.50
2	B	1384	HCY	C17-C20	-5.18	1.44	1.53
2	C	1384	HCY	C6-C5	5.14	1.59	1.50
2	C	1384	HCY	C17-C20	-5.14	1.44	1.53
2	C	1384	HCY	C13-C14	-5.04	1.45	1.54
2	D	1384	HCY	C17-C20	-5.01	1.44	1.53
2	D	1384	HCY	C12-C13	-3.59	1.47	1.53
2	C	1384	HCY	C12-C13	-3.50	1.47	1.53
2	B	1384	HCY	C12-C13	-3.48	1.48	1.53
2	D	1384	HCY	C8-C14	-3.41	1.47	1.53
2	C	1384	HCY	C8-C14	-3.37	1.47	1.53
2	A	1384	HCY	C8-C14	-3.35	1.47	1.53
2	B	1384	HCY	C8-C14	-3.31	1.47	1.53
2	A	1384	HCY	C12-C13	-3.04	1.48	1.53
2	A	1384	HCY	C7-C6	2.94	1.59	1.52
2	A	1384	HCY	C1-C10	2.68	1.59	1.54
2	D	1384	HCY	C1-C10	2.57	1.59	1.54
2	C	1384	HCY	C7-C6	2.55	1.58	1.52
2	B	1384	HCY	C7-C6	2.51	1.58	1.52
2	D	1384	HCY	C7-C6	2.50	1.58	1.52
2	C	1384	HCY	C16-C15	2.37	1.62	1.54
2	C	1384	HCY	C1-C10	2.37	1.58	1.54
2	B	1384	HCY	C1-C10	2.30	1.58	1.54
2	A	1384	HCY	C16-C15	2.24	1.61	1.54
2	B	1384	HCY	C16-C15	2.23	1.61	1.54
2	D	1384	HCY	C16-C15	2.23	1.61	1.54

All (91) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1384	HCY	O3-C17-C20	-24.29	75.26	107.70
2	C	1384	HCY	O3-C17-C20	-23.59	76.19	107.70
2	D	1384	HCY	O3-C17-C20	-22.89	77.13	107.70
2	B	1384	HCY	O3-C17-C20	-22.24	77.99	107.70
2	D	1384	HCY	C13-C17-C20	17.95	129.95	112.87
2	A	1384	HCY	C13-C17-C20	17.92	129.93	112.87
2	B	1384	HCY	C13-C17-C20	16.47	128.54	112.87
2	C	1384	HCY	C13-C17-C20	16.38	128.45	112.87
2	C	1384	HCY	C16-C17-C20	9.97	125.59	113.85
2	B	1384	HCY	C16-C17-C20	9.70	125.28	113.85
2	B	1384	HCY	O3-C17-C16	-9.49	88.57	110.34
2	B	1384	HCY	C21-C20-C17	9.23	128.70	117.76
2	D	1384	HCY	O3-C17-C16	-8.91	89.91	110.34
2	C	1384	HCY	O3-C17-C16	-8.73	90.31	110.34
2	A	1384	HCY	O3-C17-C16	-8.62	90.58	110.34
2	D	1384	HCY	C16-C17-C20	8.59	123.97	113.85
2	C	1384	HCY	C21-C20-C17	8.57	127.93	117.76
2	A	1384	HCY	C16-C17-C20	8.01	123.28	113.85
2	D	1384	HCY	C21-C20-C17	7.83	127.05	117.76
2	A	1384	HCY	C21-C20-C17	5.95	124.81	117.76
2	D	1384	HCY	C2-C3-C4	5.89	125.81	116.74
2	C	1384	HCY	C17-C13-C14	5.86	106.33	99.89
2	C	1384	HCY	C18-C13-C17	-5.84	102.17	109.14
2	D	1384	HCY	C17-C13-C14	5.81	106.27	99.89
2	A	1384	HCY	O3-C17-C13	-5.76	94.74	108.09
2	D	1384	HCY	O3-C17-C13	-5.72	94.81	108.09
2	A	1384	HCY	C18-C13-C17	-5.64	102.41	109.14
2	B	1384	HCY	C18-C13-C17	-5.57	102.50	109.14
2	A	1384	HCY	C2-C3-C4	5.55	125.29	116.74
2	A	1384	HCY	C17-C13-C14	5.51	105.95	99.89
2	B	1384	HCY	C17-C13-C14	5.31	105.73	99.89
2	B	1384	HCY	C2-C3-C4	5.09	124.58	116.74
2	B	1384	HCY	O3-C17-C13	-5.08	96.30	108.09
2	C	1384	HCY	C7-C6-C5	-5.04	102.44	111.93
2	D	1384	HCY	C18-C13-C17	-4.97	103.21	109.14
2	D	1384	HCY	C7-C6-C5	-4.75	103.00	111.93
2	D	1384	HCY	C15-C14-C8	-4.42	111.80	119.08
2	B	1384	HCY	C7-C6-C5	-4.42	103.62	111.93
2	C	1384	HCY	O3-C17-C13	-4.38	97.92	108.09
2	C	1384	HCY	C2-C3-C4	4.31	123.37	116.74
2	A	1384	HCY	C15-C14-C8	-4.29	112.02	119.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1384	HCY	O4-C20-C17	-4.20	115.67	122.20
2	B	1384	HCY	O4-C20-C17	-4.19	115.68	122.20
2	B	1384	HCY	C15-C14-C8	-3.99	112.50	119.08
2	D	1384	HCY	O4-C20-C17	-3.89	116.15	122.20
2	A	1384	HCY	C2-C1-C10	3.82	120.62	113.45
2	D	1384	HCY	C2-C1-C10	3.73	120.45	113.45
2	A	1384	HCY	C15-C14-C13	3.51	108.44	103.73
2	C	1384	HCY	C1-C2-C3	-3.48	104.16	111.62
2	C	1384	HCY	C15-C14-C8	-3.30	113.64	119.08
2	B	1384	HCY	C6-C5-C10	3.29	122.83	116.77
2	A	1384	HCY	C7-C6-C5	-3.26	105.79	111.93
2	B	1384	HCY	C12-C13-C14	3.19	110.86	108.03
2	C	1384	HCY	C12-C13-C14	3.17	110.84	108.03
2	A	1384	HCY	O4-C20-C17	-3.05	117.46	122.20
2	A	1384	HCY	C6-C7-C8	3.01	117.14	111.69
2	C	1384	HCY	C13-C12-C11	-2.94	109.62	113.84
2	B	1384	HCY	C1-C2-C3	-2.92	105.36	111.62
2	D	1384	HCY	C6-C5-C10	2.85	122.03	116.77
2	B	1384	HCY	C13-C12-C11	-2.79	109.84	113.84
2	D	1384	HCY	C1-C10-C9	-2.72	105.16	109.38
2	D	1384	HCY	C15-C14-C13	2.69	107.33	103.73
2	C	1384	HCY	C6-C5-C10	2.54	121.46	116.77
2	B	1384	HCY	C15-C14-C13	2.53	107.12	103.73
2	C	1384	HCY	C15-C14-C13	2.46	107.03	103.73
2	D	1384	HCY	O1-C3-C4	-2.45	116.98	121.68
2	A	1384	HCY	C1-C10-C9	-2.40	105.66	109.38
2	B	1384	HCY	C7-C8-C14	-2.40	107.99	112.08
2	D	1384	HCY	C12-C13-C14	2.39	110.15	108.03
2	A	1384	HCY	C16-C17-C13	2.36	105.41	103.20
2	D	1384	HCY	C10-C9-C11	-2.35	112.06	114.47
2	B	1384	HCY	C6-C5-C4	-2.35	116.94	120.87
2	B	1384	HCY	C16-C17-C13	2.30	105.36	103.20
2	C	1384	HCY	C7-C8-C14	-2.29	108.17	112.08
2	A	1384	HCY	C19-C10-C5	-2.26	104.68	108.34
2	C	1384	HCY	C16-C17-C13	2.26	105.32	103.20
2	A	1384	HCY	O1-C3-C4	-2.20	117.46	121.68
2	B	1384	HCY	C19-C10-C9	2.18	116.26	112.65
2	D	1384	HCY	C6-C5-C4	-2.17	117.24	120.87
2	B	1384	HCY	O4-C20-C21	-2.16	115.61	119.71
2	B	1384	HCY	C9-C10-C5	2.15	111.83	108.21
2	B	1384	HCY	C12-C13-C17	-2.15	114.58	116.16
2	C	1384	HCY	C12-C11-C9	-2.13	109.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1384	HCY	O1-C3-C4	-2.13	117.59	121.68
2	A	1384	HCY	C7-C8-C14	-2.13	108.45	112.08
2	B	1384	HCY	C12-C11-C9	-2.12	109.70	112.60
2	D	1384	HCY	O1-C3-C2	-2.11	117.21	121.57
2	A	1384	HCY	O1-C3-C2	-2.10	117.22	121.57
2	C	1384	HCY	C15-C16-C17	-2.09	102.40	106.00
2	C	1384	HCY	C12-C13-C17	-2.09	114.62	116.16
2	B	1384	HCY	C2-C1-C10	2.03	117.25	113.45

There are no chirality outliers.

All (23) torsion outliers are listed below:

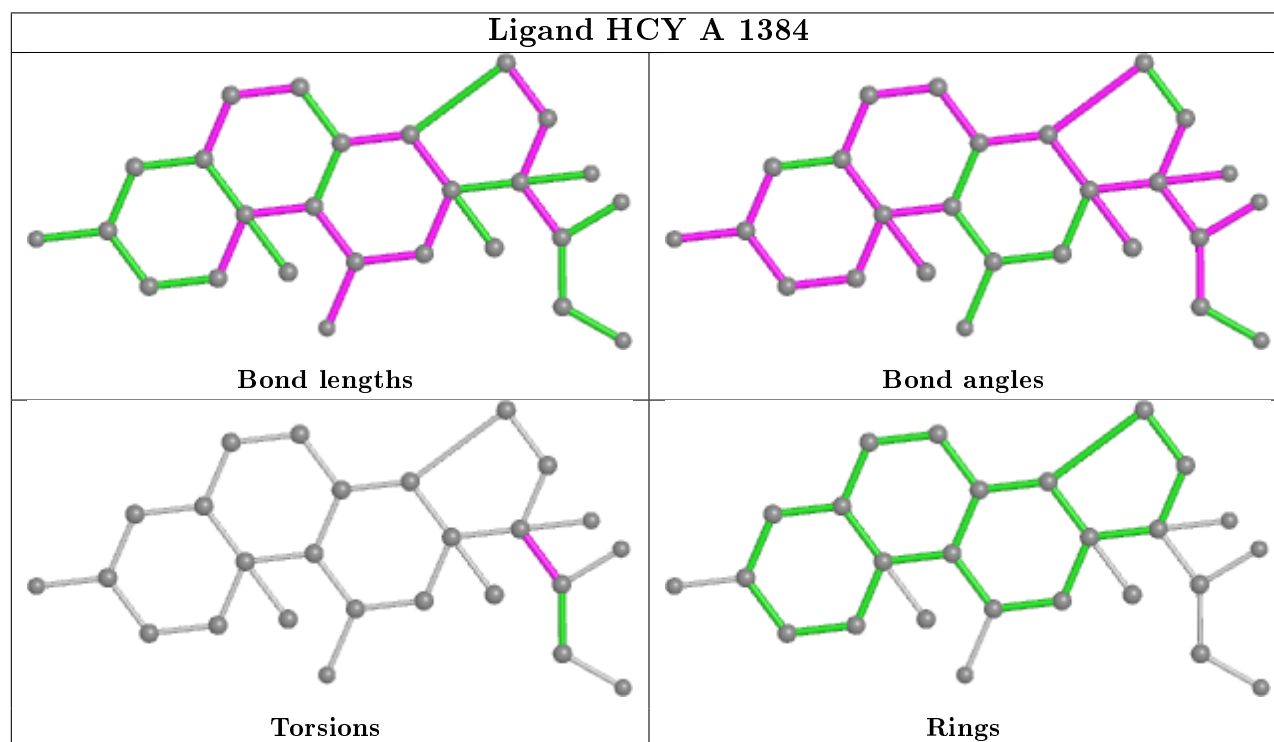
Mol	Chain	Res	Type	Atoms
2	A	1384	HCY	C13-C17-C20-C21
2	A	1384	HCY	C13-C17-C20-O4
2	A	1384	HCY	O3-C17-C20-C21
2	A	1384	HCY	O3-C17-C20-O4
2	C	1384	HCY	C13-C17-C20-C21
2	C	1384	HCY	C13-C17-C20-O4
2	C	1384	HCY	C16-C17-C20-C21
2	C	1384	HCY	C16-C17-C20-O4
2	B	1384	HCY	C13-C17-C20-C21
2	B	1384	HCY	C13-C17-C20-O4
2	B	1384	HCY	C17-C20-C21-O5
2	B	1384	HCY	O4-C20-C21-O5
2	D	1384	HCY	C13-C17-C20-C21
2	D	1384	HCY	C13-C17-C20-O4
2	B	1384	HCY	O3-C17-C20-C21
2	B	1384	HCY	C16-C17-C20-O4
2	D	1384	HCY	O4-C20-C21-O5
2	D	1384	HCY	O3-C17-C20-C21
2	D	1384	HCY	C17-C20-C21-O5
2	D	1384	HCY	C16-C17-C20-O4
2	C	1384	HCY	O4-C20-C21-O5
2	B	1384	HCY	C16-C17-C20-C21
2	D	1384	HCY	C16-C17-C20-C21

There are no ring outliers.

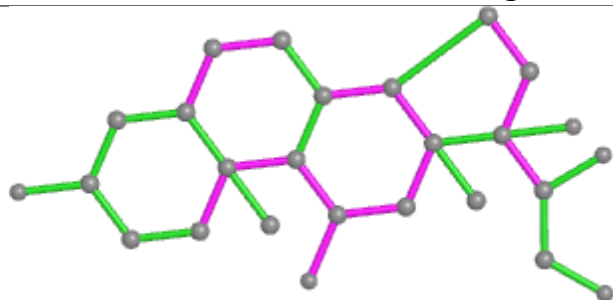
4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1384	HCY	3	0
2	C	1384	HCY	3	0
2	B	1384	HCY	5	0
2	D	1384	HCY	6	0

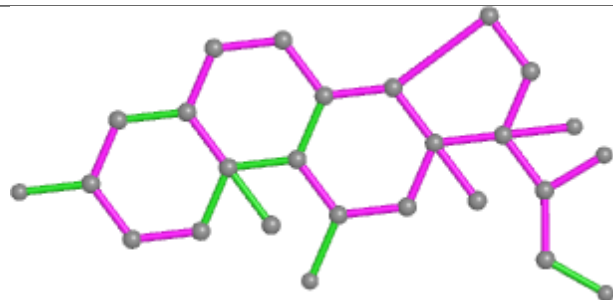
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



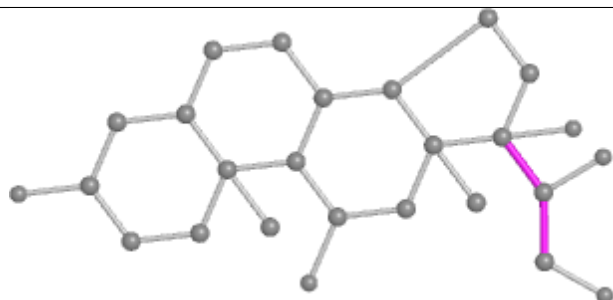
## Ligand HCY C 1384



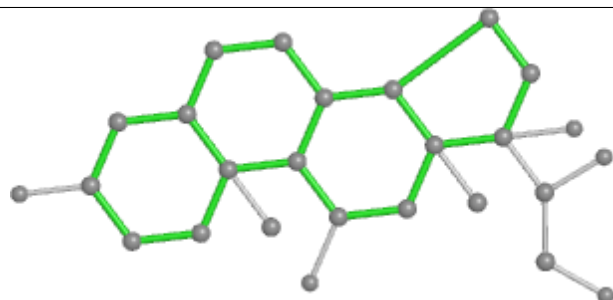
Bond lengths



Bond angles

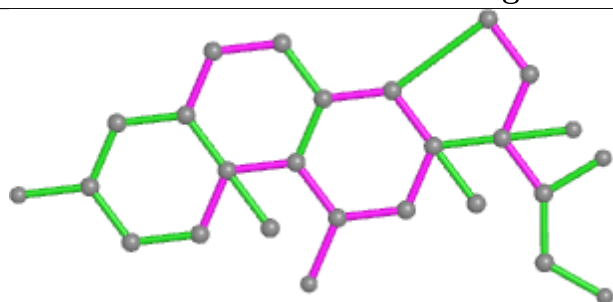


Torsions

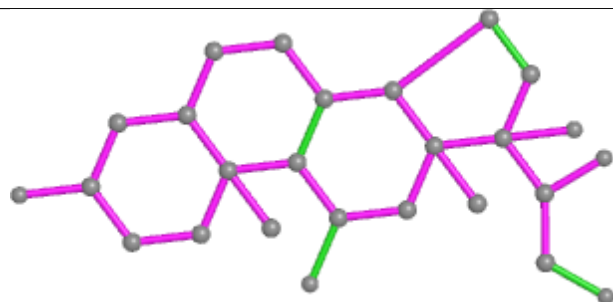


Rings

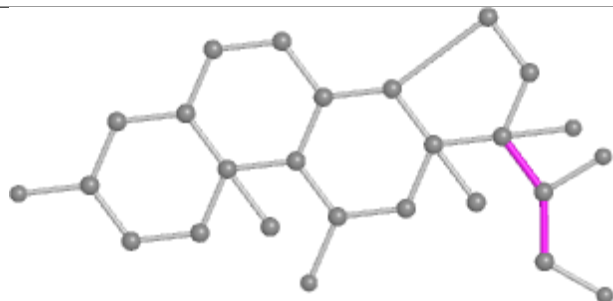
## Ligand HCY B 1384



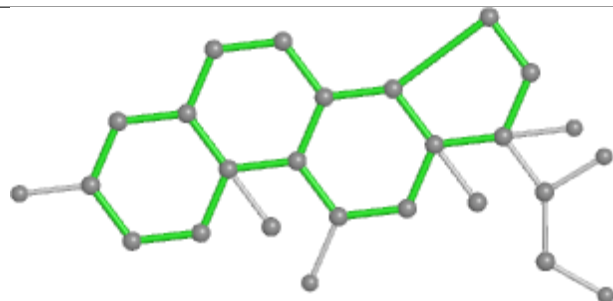
Bond lengths



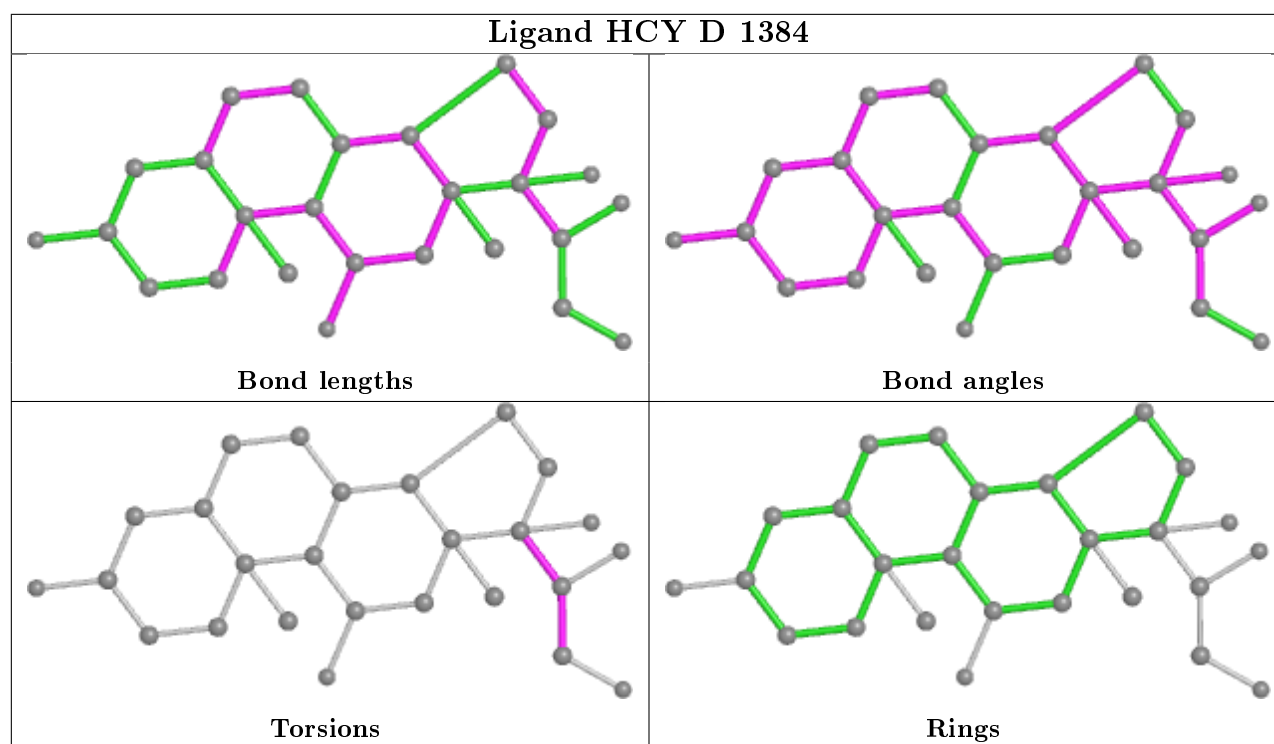
Bond angles



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<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	367/373 (98%)	0.06	5 (1%) 75 77	33, 58, 94, 149	0
1	B	362/373 (97%)	0.19	10 (2%) 53 54	36, 61, 95, 129	1 (0%)
1	C	363/373 (97%)	0.22	9 (2%) 57 59	37, 66, 97, 128	1 (0%)
1	D	356/373 (95%)	0.70	42 (11%) 4 3	45, 83, 114, 127	1 (0%)
All	All	1448/1492 (97%)	0.29	66 (4%) 32 31	33, 66, 106, 149	3 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	GLY	6.8
1	C	351	LYS	5.9
1	D	241	VAL	5.8
1	D	164	PHE	4.8
1	D	220	TYR	4.5
1	D	75	LEU	4.5
1	D	283	THR	4.4
1	D	236	VAL	4.2
1	D	178	TYR	4.0
1	D	182	LYS	3.9
1	D	195	ARG	3.9
1	D	16	GLY	3.9
1	D	383	VAL	3.8
1	D	249	GLY	3.8
1	D	136	MET	3.8
1	D	79	SER	3.6
1	A	138	PHE	3.5
1	B	203	GLU	3.5
1	D	180	PHE	3.5
1	D	287	VAL	3.3
1	D	218	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	75	LEU	3.3
1	D	233	MET	3.2
1	D	73	PHE	3.1
1	B	202	ASP	3.1
1	D	132	GLU	3.1
1	C	101	LEU	3.0
1	D	282	VAL	3.0
1	D	284	ILE	3.0
1	C	315	ASP	2.9
1	D	94	PHE	2.9
1	D	205	THR	2.8
1	A	98	ASP	2.8
1	D	103	MET	2.7
1	D	38	LYS	2.7
1	C	75	LEU	2.7
1	D	276	ASP	2.7
1	D	315	ASP	2.7
1	D	36	SER	2.6
1	D	280	PRO	2.6
1	D	372	SER	2.6
1	D	324	VAL	2.5
1	B	32	LEU	2.4
1	D	328	VAL	2.4
1	D	105	MET	2.4
1	C	111	LEU	2.4
1	D	224	SER	2.4
1	B	351	LYS	2.4
1	C	166	GLY	2.3
1	D	209	VAL	2.3
1	D	160	ILE	2.2
1	D	229	GLN	2.2
1	B	248	LYS	2.2
1	D	92	GLN	2.2
1	A	369	PHE	2.2
1	B	316	ALA	2.2
1	D	78	ARG	2.1
1	D	339	ALA	2.1
1	A	203	GLU	2.1
1	C	173	LEU	2.1
1	B	52	LEU	2.1
1	B	172	ILE	2.1
1	C	312	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	249	GLY	2.1
1	B	115	LEU	2.1
1	D	288	TYR	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

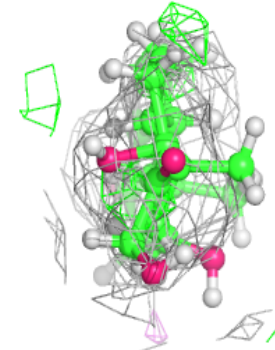
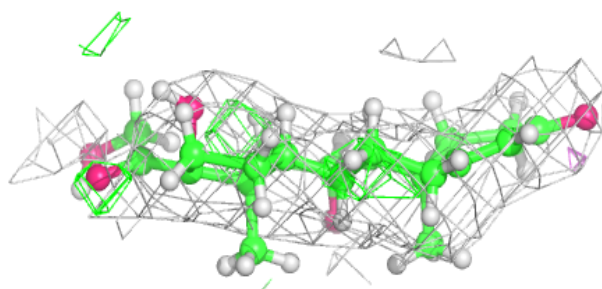
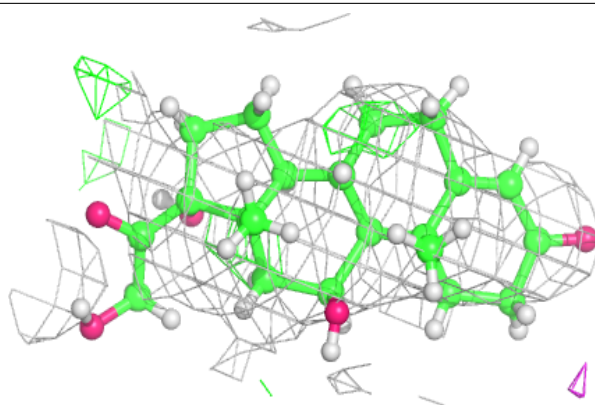
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HCY	D	1384	26/26	0.70	0.31	91,207,367,377	0
2	HCY	B	1384	26/26	0.82	0.24	75,103,240,265	0
2	HCY	A	1384	26/26	0.82	0.36	93,125,180,262	0
2	HCY	C	1384	26/26	0.93	0.16	60,79,94,101	0

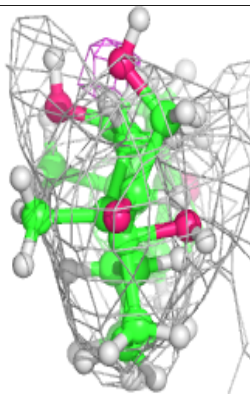
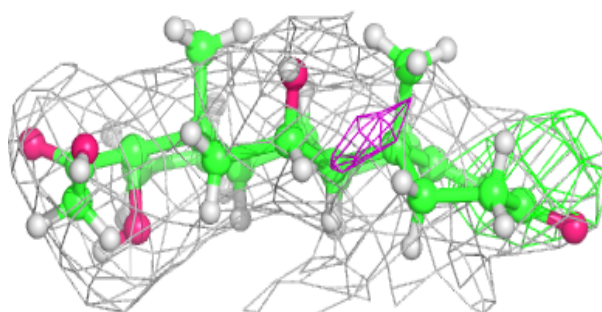
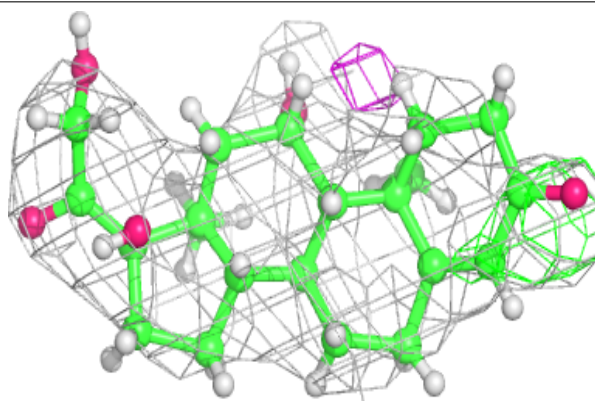
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around HCY D 1384:**

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

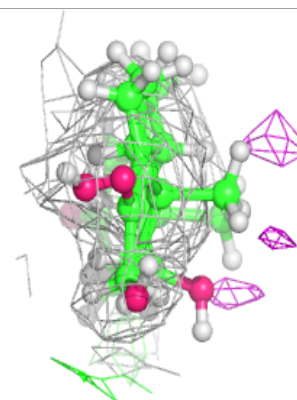
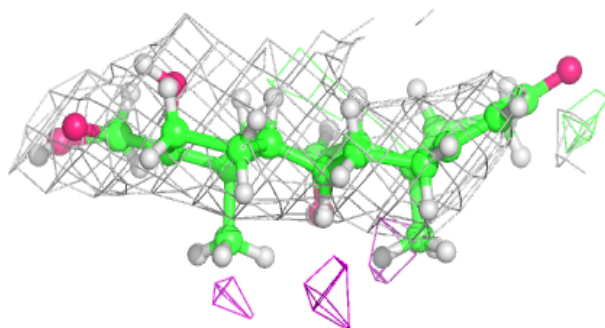
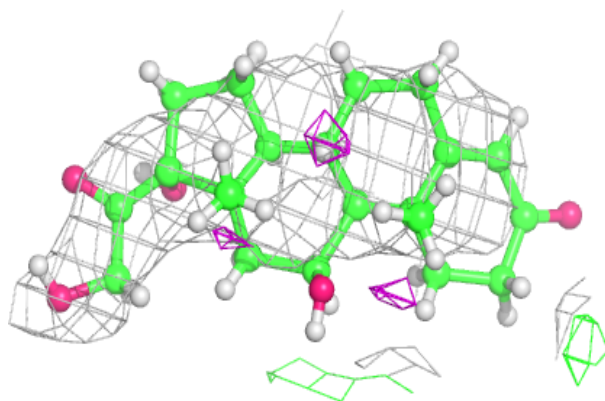
**Electron density around HCY B 1384:**

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

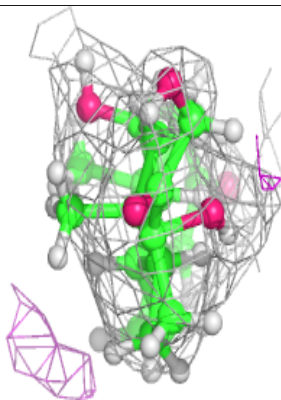
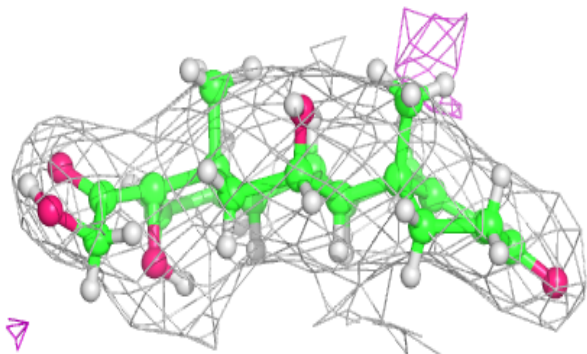
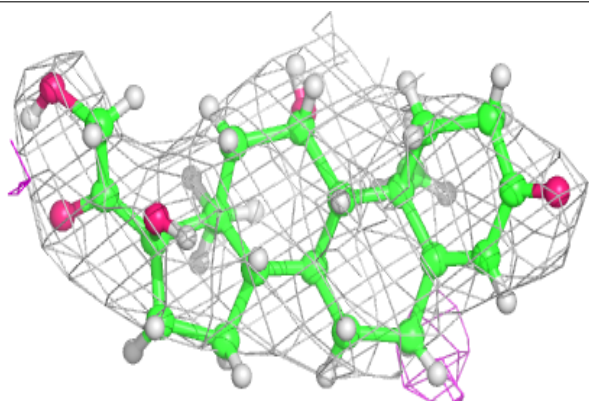


**Electron density around HCY A 1384:**

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

**Electron density around HCY C 1384:**

$2mF_o-DF_c$  (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.