



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:12 AM GMT

PDB ID : 3DOY  
Title : Crystal structure of (3R)-Hydroxyacyl-Acyl Carrier Protein Dehydratase (FabZ) from Helicobacter pylori in complex with compound 3i  
Authors : Zhang, L.; He, L.; Liu, X.; Liu, H.; Shen, X.; Jiang, H.  
Deposited on : 2008-07-07  
Resolution : 2.40 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

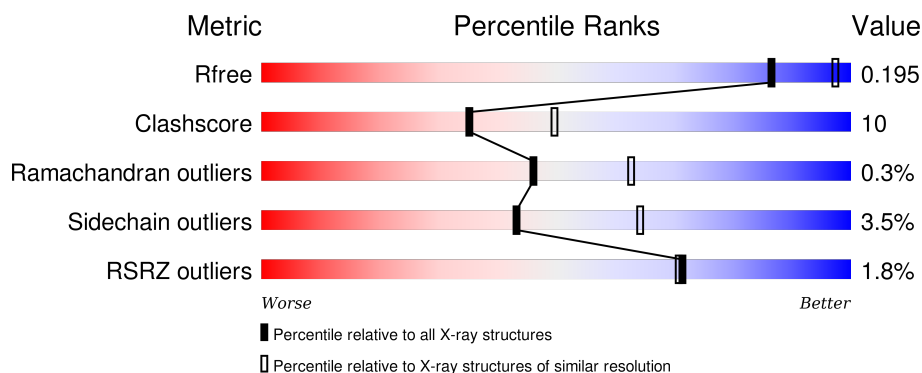
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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	159	<div> <div>0%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>• •</div> </div> </div>
1	B	159	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>• 6%</div> </div> </div>
1	C	159	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>• 6%</div> </div> </div>
1	D	159	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• 5%</div> </div> </div>
1	E	159	<div> <div>0%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	159	 % 79% 13% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BEN	A	2005	-	-	-	X
3	BEN	B	2007	-	-	-	X
3	BEN	B	2009	-	-	X	X
3	BEN	C	2004	-	-	-	X
3	BEN	E	2008	-	-	-	X
4	2BE	A	3001	-	-	-	X
4	2BE	C	3002	-	-	X	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7838 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 (3R)-hydroxymyristoyl-acyl carrier protein dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1224	803	203	213	5			
1	B	149	Total	C	N	O	S	0	0	0
			1198	787	199	207	5			
1	C	150	Total	C	N	O	S	0	0	0
			1207	792	201	209	5			
1	D	151	Total	C	N	O	S	0	0	0
			1216	797	202	212	5			
1	E	151	Total	C	N	O	S	0	0	0
			1216	797	202	212	5			
1	F	148	Total	C	N	O	S	0	0	0
			1192	784	198	205	5			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

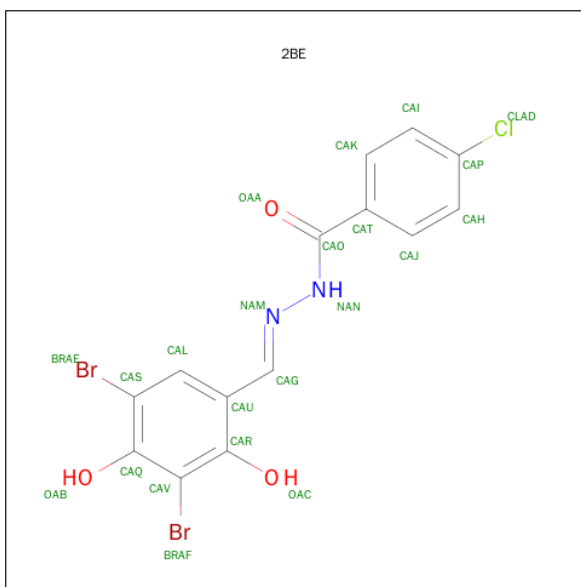
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cl	0	0
			1	1		
2	E	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		
2	F	1	Total	Cl	0	0
			1	1		

- Molecule 3 is BENZAMIDINE (three-letter code: BEN) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	7	2		
3	A	1	Total	C	N	0	0
			9	7	2		
3	B	1	Total	C	N	0	0
			9	7	2		
3	B	1	Total	C	N	0	0
			9	7	2		
3	C	1	Total	C	N	0	0
			9	7	2		
3	E	1	Total	C	N	0	0
			9	7	2		

- Molecule 4 is 4-CHLORO-N'-[(1E)-(3,5-DIBROMO-2,4-DIHYDROXYPHENYL)METHYL IDENE]BENZOHYDRAZIDE (three-letter code: 2BE) (formula: C<sub>14</sub>H<sub>9</sub>Br<sub>2</sub>ClN<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 22	Br 2	C 14	Cl 1	N 2	O 3	0	0
4	C	1	Total 22	Br 2	C 14	Cl 1	N 2	O 3	0	0

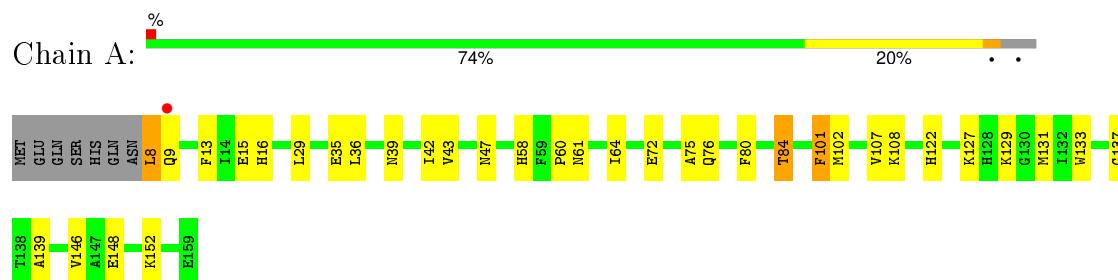
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	82	Total O 82 82	0	0
5	B	97	Total O 97 97	0	0
5	C	78	Total O 78 78	0	0
5	D	70	Total O 70 70	0	0
5	E	84	Total O 84 84	0	0
5	F	70	Total O 70 70	0	0

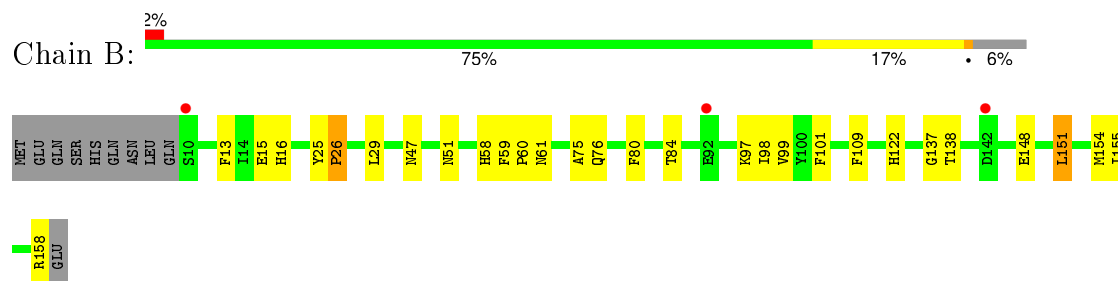
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

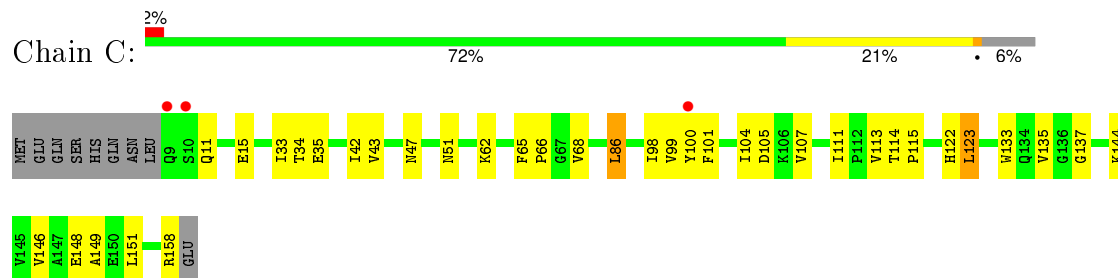
- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase



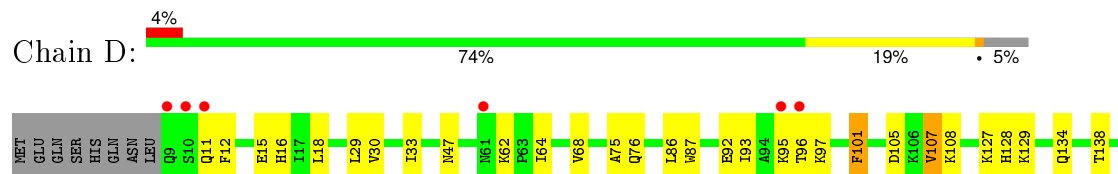
- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase



- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase

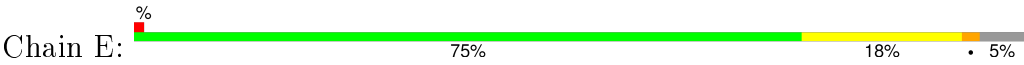


- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase

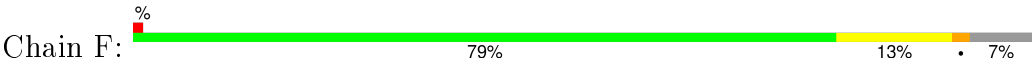




● Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase



● Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.97Å 100.37Å 186.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.0 (15.00-2.40) 97.0 (20.00-2.40)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.41Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.200 , 0.238 0.200 , 0.195	Depositor DCC
$R_{free}$ test set	2713 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 53397 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7838	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.10 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6429e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2BE, BEN, CL

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	0.42	0/1255	0.63	0/1697
1	B	0.41	0/1229	0.61	0/1663
1	C	0.40	0/1238	0.62	0/1675
1	D	0.42	0/1247	0.63	0/1686
1	E	0.40	0/1247	0.64	0/1686
1	F	0.40	0/1223	0.64	0/1655
All	All	0.41	0/7439	0.63	0/10062

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	1224	0	1243	26	0
1	B	1198	0	1218	24	0
1	C	1207	0	1226	30	0
1	D	1216	0	1232	27	0
1	E	1216	0	1232	25	0
1	F	1192	0	1213	22	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	18	0	14	1	0
3	B	18	0	14	5	0
3	C	9	0	7	0	0
3	E	9	0	7	0	0
4	A	22	0	7	3	0
4	C	22	0	7	8	0
5	A	82	0	0	1	0
5	B	97	0	0	2	0
5	C	78	0	0	5	0
5	D	70	0	0	3	0
5	E	84	0	0	2	0
5	F	70	0	0	3	0
All	All	7838	0	7420	145	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 10.

All (145) 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)
4:C:3002:2BE:HAG	4:C:3002:2BE:CAK	1.43	1.46
4:C:3002:2BE:CAG	4:C:3002:2BE:HAK	1.56	1.35
4:A:3001:2BE:HAG	4:A:3001:2BE:OAA	1.50	1.08
1:B:98:ILE:HD12	3:B:2009:BEN:HN21	1.27	0.99
1:A:8:LEU:HD11	1:A:84:THR:HG23	1.51	0.92
4:C:3002:2BE:CAG	4:C:3002:2BE:CAK	2.30	0.90
4:C:3002:2BE:HAK	4:C:3002:2BE:HAG	0.87	0.87
1:D:29:LEU:H	1:D:76:GLN:HE22	1.20	0.86
1:B:13:PHE:H	1:B:16:HIS:HD2	1.19	0.85
1:B:29:LEU:H	1:B:76:GLN:HE22	1.25	0.84
1:A:29:LEU:H	1:A:76:GLN:HE22	1.26	0.82
1:F:37:GLN:HB3	1:F:40:GLN:HE21	1.49	0.77
1:A:13:PHE:H	1:A:16:HIS:HD2	1.33	0.76
1:D:93:ILE:O	1:D:96:THR:HG22	1.86	0.76
1:C:86:LEU:HD11	1:C:133:TRP:HZ2	1.51	0.75
1:C:111:ILE:O	1:C:146:VAL:HG13	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:GLU:HB3	5:D:3379:HOH:O	1.86	0.74
1:B:99:VAL:HG22	1:B:155:ILE:HG12	1.70	0.73
1:C:62:LYS:HD2	5:C:3076:HOH:O	1.87	0.73
1:B:47:ASN:HB3	1:F:47:ASN:HB3	1.71	0.73
1:D:96:THR:O	1:D:97:LYS:HG3	1.89	0.72
1:C:47:ASN:HB3	1:E:47:ASN:HB3	1.70	0.71
1:B:98:ILE:HD12	3:B:2009:BEN:N2	2.03	0.69
1:E:118:ARG:HD2	5:E:3164:HOH:O	1.93	0.69
1:E:35:GLU:HG2	1:E:43:VAL:HB	1.73	0.69
1:A:80:PHE:O	1:A:84:THR:HB	1.95	0.67
1:D:29:LEU:N	1:D:76:GLN:HE22	1.90	0.67
1:C:15:GLU:HB3	5:C:3036:HOH:O	1.94	0.66
5:C:3076:HOH:O	1:E:15:GLU:HG2	1.95	0.65
4:A:3001:2BE:CAG	4:A:3001:2BE:OAA	2.30	0.65
1:E:107:VAL:HG22	1:F:104:ILE:HB	1.77	0.65
1:D:29:LEU:H	1:D:76:GLN:NE2	1.95	0.64
1:B:13:PHE:H	1:B:16:HIS:CD2	2.10	0.63
1:D:30:VAL:HG23	1:D:76:GLN:HE21	1.64	0.62
1:E:107:VAL:CG2	1:F:104:ILE:HB	2.28	0.62
1:A:102:MET:SD	1:A:152:LYS:HE3	2.40	0.61
1:D:87:TRP:CH2	1:D:97:LYS:HE2	2.38	0.59
1:C:98:ILE:HD11	1:C:100:TYR:CZ	2.39	0.58
1:A:35:GLU:HG2	1:A:43:VAL:HB	1.85	0.58
1:C:104:ILE:HB	1:D:107:VAL:HG22	1.86	0.58
1:F:37:GLN:HB3	1:F:40:GLN:NE2	2.17	0.58
1:D:95:LYS:HE2	5:D:3322:HOH:O	2.03	0.56
1:A:127:LYS:HZ3	1:A:129:LYS:HE2	1.71	0.56
1:C:104:ILE:HB	1:D:107:VAL:CG2	2.36	0.55
1:D:127:LYS:HE2	1:D:129:LYS:CD	2.37	0.55
1:D:127:LYS:HG2	1:D:128:HIS:N	2.20	0.55
1:D:11:GLN:HG3	1:D:33:ILE:O	2.06	0.55
1:D:92:GLU:HG3	5:D:3322:HOH:O	2.08	0.54
1:B:98:ILE:CD1	3:B:2009:BEN:HN21	2.11	0.54
1:D:127:LYS:HE2	1:D:129:LYS:HD3	1.90	0.54
1:A:60:PRO:O	1:A:61:ASN:HB2	2.08	0.54
1:E:62:LYS:HD3	1:F:98:ILE:HD13	1.89	0.53
1:C:86:LEU:HD11	1:C:133:TRP:CZ2	2.37	0.53
1:C:99:VAL:H	4:C:3002:2BE:CAL	2.21	0.53
1:A:72:GLU:O	1:A:76:GLN:HG3	2.09	0.53
1:C:158:ARG:HD3	4:C:3002:2BE:CLAD	2.46	0.53
1:E:40:GLN:HG2	5:E:3458:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LEU:HD11	1:A:84:THR:CG2	2.32	0.52
1:D:96:THR:C	1:D:97:LYS:HG3	2.30	0.52
1:F:60:PRO:O	1:F:61:ASN:HB2	2.09	0.52
1:A:35:GLU:CG	1:A:43:VAL:HB	2.41	0.51
1:B:151:LEU:N	1:B:151:LEU:HD12	2.26	0.51
4:A:3001:2BE:HAI	5:B:3370:HOH:O	2.10	0.51
1:F:82:ALA:O	1:F:86:LEU:HB2	2.11	0.51
1:E:36:LEU:HD13	1:E:42:ILE:HD12	1.92	0.50
1:A:29:LEU:H	1:A:76:GLN:NE2	2.04	0.50
1:C:86:LEU:CD1	1:C:133:TRP:HZ2	2.21	0.49
1:E:104:ILE:HB	1:F:107:VAL:HG22	1.94	0.49
1:A:9:GLN:HB3	5:A:3409:HOH:O	2.12	0.49
1:E:60:PRO:O	1:E:61:ASN:HB2	2.13	0.49
1:B:98:ILE:HA	3:B:2009:BEN:H2	1.94	0.49
1:A:47:ASN:HB3	1:D:47:ASN:HB3	1.94	0.49
1:F:37:GLN:HE21	1:F:40:GLN:NE2	2.10	0.49
1:B:122:HIS:O	1:B:137:GLY:HA3	2.13	0.49
1:F:92:GLU:O	1:F:95:LYS:HG2	2.13	0.48
1:D:158:ARG:O	1:D:159:GLU:HB2	2.12	0.48
1:C:101:PHE:HE1	4:C:3002:2BE:BRAF	2.51	0.48
5:C:3076:HOH:O	1:E:15:GLU:CG	2.57	0.48
1:D:62:LYS:HD2	1:D:64:ILE:HD11	1.95	0.48
1:F:158:ARG:HH11	1:F:158:ARG:HG2	1.79	0.48
1:E:12:PHE:HB3	1:E:16:HIS:HB2	1.96	0.47
1:A:75:ALA:HB2	1:A:101:PHE:CZ	2.50	0.47
1:B:138:THR:HG22	1:B:148:GLU:HB3	1.94	0.47
1:C:98:ILE:HA	4:C:3002:2BE:HAL	1.97	0.47
1:E:62:LYS:CD	1:F:98:ILE:HD13	2.45	0.47
1:C:107:VAL:HG22	1:C:149:ALA:CB	2.45	0.47
1:B:58:HIS:N	1:B:59:PHE:HA	2.29	0.47
1:D:93:ILE:O	1:D:96:THR:CG2	2.60	0.47
1:D:75:ALA:HB2	1:D:101:PHE:CZ	2.49	0.47
1:C:122:HIS:O	1:C:137:GLY:HA3	2.15	0.47
1:C:68:VAL:HB	1:D:68:VAL:HB	1.97	0.46
1:B:15:GLU:CG	5:F:3448:HOH:O	2.63	0.46
1:B:97:LYS:O	3:B:2009:BEN:H3	2.16	0.46
1:E:104:ILE:HB	1:F:107:VAL:CG2	2.45	0.46
1:B:29:LEU:N	1:B:76:GLN:HE22	2.03	0.46
1:A:9:GLN:HA	1:A:9:GLN:HE21	1.80	0.45
1:B:15:GLU:HG3	5:F:3448:HOH:O	2.17	0.45
1:E:98:ILE:HD13	1:F:62:LYS:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LEU:H	1:B:76:GLN:NE2	2.05	0.45
1:A:131:MET:HB2	3:A:2005:BEN:N1	2.32	0.45
1:C:107:VAL:HG22	1:C:149:ALA:HB2	1.98	0.45
1:F:158:ARG:NH1	5:F:3475:HOH:O	2.45	0.45
1:E:86:LEU:HD13	1:E:133:TRP:HZ2	1.82	0.44
1:C:35:GLU:HB2	1:C:43:VAL:HB	2.00	0.44
1:D:12:PHE:HB3	1:D:16:HIS:HB2	1.98	0.44
1:A:29:LEU:N	1:A:76:GLN:HE22	2.06	0.44
1:B:25:TYR:CE1	1:B:26:PRO:HB3	2.53	0.44
1:D:30:VAL:HG23	1:D:76:GLN:NE2	2.32	0.44
1:A:107:VAL:HA	1:A:148:GLU:O	2.18	0.43
1:E:68:VAL:HB	1:F:68:VAL:HB	1.99	0.43
1:E:122:HIS:O	1:E:137:GLY:HA3	2.17	0.43
1:A:122:HIS:O	1:A:137:GLY:HA3	2.18	0.43
1:C:104:ILE:HG12	1:C:151:LEU:CD2	2.48	0.43
1:A:139:ALA:O	1:A:146:VAL:HG22	2.19	0.43
1:F:33:ILE:HD12	1:F:42:ILE:HD11	1.99	0.43
1:A:108:LYS:HE2	5:B:3208:HOH:O	2.17	0.43
1:F:92:GLU:CD	1:F:95:LYS:HE3	2.39	0.43
1:A:39:ASN:HD22	1:A:133:TRP:HH2	1.66	0.43
1:A:101:PHE:HB3	1:B:109:PHE:CD1	2.53	0.43
1:C:114:THR:HB	1:C:115:PRO:HD2	2.00	0.43
1:A:58:HIS:ND1	1:A:64:ILE:O	2.47	0.43
1:C:33:ILE:HD12	1:C:42:ILE:HD11	1.99	0.43
1:C:123:LEU:HD23	1:C:135:VAL:HG22	2.00	0.43
1:E:83:PHE:CD2	1:E:83:PHE:C	2.92	0.42
1:D:138:THR:HG22	1:D:148:GLU:HG2	2.00	0.42
1:B:75:ALA:HB1	1:B:101:PHE:CE1	2.53	0.42
1:B:80:PHE:CE2	1:B:84:THR:HG21	2.55	0.42
1:B:25:TYR:HA	1:B:26:PRO:HA	1.83	0.42
1:F:97:LYS:HA	1:F:156:ALA:O	2.19	0.42
1:C:107:VAL:HA	1:C:148:GLU:O	2.20	0.42
1:E:107:VAL:HA	1:E:148:GLU:O	2.20	0.41
1:E:49:THR:HG23	1:E:52:GLU:HG3	2.01	0.41
1:C:34:THR:HG21	5:C:3022:HOH:O	2.20	0.41
1:B:60:PRO:O	1:B:61:ASN:HB2	2.21	0.41
1:C:144:LYS:HB2	1:C:144:LYS:HE3	1.85	0.41
1:E:134:GLN:HG2	1:E:152:LYS:HB2	2.02	0.41
1:C:65:PHE:HA	1:C:66:PRO:HD3	1.92	0.41
1:D:134:GLN:HE21	1:D:134:GLN:HB2	1.71	0.41
1:A:36:LEU:HD23	1:A:42:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:THR:HB	1:C:115:PRO:CD	2.51	0.40
1:C:113:VAL:HG22	1:C:146:VAL:HG11	2.03	0.40
1:F:122:HIS:C	1:F:123:LEU:HD22	2.42	0.40
1:C:86:LEU:CD1	1:C:133:TRP:CZ2	3.03	0.40
1:E:107:VAL:HG21	1:F:104:ILE:HB	2.03	0.40
1:E:84:THR:O	1:E:88:GLY:HA2	2.22	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	150/159 (94%)	142 (95%)	8 (5%)	0	100	100
1	B	147/159 (92%)	141 (96%)	5 (3%)	1 (1%)	26	38
1	C	148/159 (93%)	141 (95%)	6 (4%)	1 (1%)	26	38
1	D	149/159 (94%)	145 (97%)	4 (3%)	0	100	100
1	E	149/159 (94%)	140 (94%)	8 (5%)	1 (1%)	26	38
1	F	146/159 (92%)	141 (97%)	5 (3%)	0	100	100
All	All	889/954 (93%)	850 (96%)	36 (4%)	3 (0%)	46	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	51	ASN
1	B	51	ASN
1	E	51	ASN

### 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	131/138 (95%)	127 (97%)	4 (3%)	47	69
1	B	128/138 (93%)	124 (97%)	4 (3%)	47	69
1	C	129/138 (94%)	125 (97%)	4 (3%)	47	69
1	D	130/138 (94%)	124 (95%)	6 (5%)	33	51
1	E	130/138 (94%)	126 (97%)	4 (3%)	47	69
1	F	127/138 (92%)	122 (96%)	5 (4%)	39	59
All	All	775/828 (94%)	748 (96%)	27 (4%)	43	64

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	15	GLU
1	A	84	THR
1	A	101	PHE
1	B	26	PRO
1	B	151	LEU
1	B	154	MET
1	B	158	ARG
1	C	11	GLN
1	C	86	LEU
1	C	105	ASP
1	C	123	LEU
1	D	18	LEU
1	D	86	LEU
1	D	101	PHE
1	D	105	ASP
1	D	107	VAL
1	D	108	LYS
1	E	86	LEU
1	E	101	PHE
1	E	107	VAL
1	E	134	GLN

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Mol	Chain	Res	Type
1	F	15	GLU
1	F	86	LEU
1	F	101	PHE
1	F	107	VAL
1	F	158	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	16	HIS
1	A	37	GLN
1	A	39	ASN
1	A	51	ASN
1	A	76	GLN
1	A	134	GLN
1	B	16	HIS
1	B	37	GLN
1	B	40	GLN
1	B	51	ASN
1	B	76	GLN
1	B	134	GLN
1	C	9	GLN
1	C	37	GLN
1	C	51	ASN
1	D	11	GLN
1	D	76	GLN
1	D	134	GLN
1	E	37	GLN
1	F	39	ASN
1	F	40	GLN
1	F	51	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BEN	A	2001	-	9,9,9	1.68	1 (11%)	9,11,11	0.56	0
3	BEN	A	2005	-	9,9,9	1.69	1 (11%)	9,11,11	0.67	0
4	2BE	A	3001	-	23,23,23	3.01	3 (13%)	30,32,32	1.27	4 (13%)
3	BEN	B	2007	-	9,9,9	1.67	1 (11%)	9,11,11	0.56	0
3	BEN	B	2009	-	9,9,9	1.68	1 (11%)	9,11,11	0.57	0
3	BEN	C	2004	-	9,9,9	1.68	1 (11%)	9,11,11	0.61	0
4	2BE	C	3002	-	23,23,23	3.06	3 (13%)	30,32,32	2.62	5 (16%)
3	BEN	E	2008	-	9,9,9	1.70	1 (11%)	9,11,11	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BEN	A	2001	-	-	0/4/4/4	0/1/1/1
3	BEN	A	2005	-	-	0/4/4/4	0/1/1/1
4	2BE	A	3001	-	-	0/10/10/10	0/2/2/2
3	BEN	B	2007	-	-	0/4/4/4	0/1/1/1
3	BEN	B	2009	-	-	0/4/4/4	0/1/1/1
3	BEN	C	2004	-	-	0/4/4/4	0/1/1/1
4	2BE	C	3002	-	-	0/10/10/10	0/2/2/2
3	BEN	E	2008	-	-	0/4/4/4	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3002	2BE	NAN-NAM	-13.39	1.23	1.38
4	A	3001	2BE	NAN-NAM	-13.30	1.23	1.38
3	E	2008	BEN	C1-C	-4.80	1.39	1.47
3	A	2005	BEN	C1-C	-4.78	1.39	1.47
3	B	2009	BEN	C1-C	-4.78	1.39	1.47
3	A	2001	BEN	C1-C	-4.75	1.39	1.47
3	C	2004	BEN	C1-C	-4.74	1.39	1.47
3	B	2007	BEN	C1-C	-4.74	1.39	1.47
4	C	3002	2BE	CAU-CAG	-3.23	1.39	1.45
4	A	3001	2BE	CAU-CAG	-3.17	1.39	1.45
4	A	3001	2BE	CAG-NAM	3.88	1.32	1.28
4	C	3002	2BE	CAG-NAM	4.16	1.32	1.28

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3002	2BE	CAU-CAG-NAM	-4.32	114.10	120.63
4	A	3001	2BE	OAA-CAO-CAT	-2.02	117.52	120.97
4	A	3001	2BE	CAR-CAU-CAG	-2.02	118.93	121.14
4	C	3002	2BE	CAU-CAR-CAV	2.19	120.47	118.13
4	A	3001	2BE	CAU-CAR-CAV	2.36	120.66	118.13
4	C	3002	2BE	CAT-CAO-NAN	3.34	120.94	116.07
4	A	3001	2BE	CAU-CAG-NAM	3.61	126.08	120.63
4	C	3002	2BE	CAG-NAM-NAN	8.15	129.31	115.86
4	C	3002	2BE	CAO-NAN-NAM	9.10	132.18	118.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2005	BEN	1	0
4	A	3001	2BE	3	0
3	B	2009	BEN	5	0
4	C	3002	2BE	8	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	152/159 (95%)	-0.56	1 (0%) 89 88	10, 16, 29, 36	0
1	B	149/159 (93%)	-0.37	3 (2%) 68 68	10, 16, 28, 38	0
1	C	150/159 (94%)	-0.37	3 (2%) 68 68	11, 18, 29, 38	0
1	D	151/159 (94%)	-0.37	7 (4%) 36 37	7, 17, 33, 40	0
1	E	151/159 (94%)	-0.54	1 (0%) 89 88	12, 17, 29, 35	0
1	F	148/159 (93%)	-0.44	1 (0%) 89 88	9, 17, 28, 35	0
All	All	901/954 (94%)	-0.44	16 (1%) 71 71	7, 17, 29, 40	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	SER	5.5
1	D	9	GLN	3.8
1	D	159	GLU	3.3
1	C	100	TYR	3.0
1	D	96	THR	2.6
1	C	10	SER	2.6
1	D	95	LYS	2.5
1	B	92	GLU	2.4
1	C	9	GLN	2.4
1	D	10	SER	2.4
1	F	142	ASP	2.2
1	B	142	ASP	2.2
1	D	11	GLN	2.2
1	E	11	GLN	2.2
1	A	9	GLN	2.2
1	D	61	ASN	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BEN	A	2005	9/9	0.86	0.34	10.54	29,30,36,37	0
4	2BE	A	3001	22/22	0.82	0.35	5.61	41,50,61,64	0
3	BEN	B	2009	9/9	0.75	0.33	4.58	23,25,29,30	0
3	BEN	B	2007	9/9	0.77	0.26	4.57	23,24,26,26	0
3	BEN	C	2004	9/9	0.89	0.27	4.49	22,23,28,29	0
4	2BE	C	3002	22/22	0.81	0.38	4.21	41,50,59,62	0
3	BEN	E	2008	9/9	0.83	0.26	3.86	30,30,32,32	0
3	BEN	A	2001	9/9	0.92	0.12	0.98	17,18,19,20	0
2	CL	F	1006	1/1	0.98	0.11	-0.17	30,30,30,30	0
2	CL	E	1005	1/1	0.98	0.07	-1.75	30,30,30,30	0
2	CL	B	1002	1/1	0.95	0.14	-	57,57,57,57	0
2	CL	C	1003	1/1	0.97	0.06	-	31,31,31,31	0
2	CL	D	1004	1/1	0.97	0.13	-	49,49,49,49	0
2	CL	A	1001	1/1	0.96	0.07	-	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.