



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2017 – 04:08 PM EDT

PDB ID : 2GLP  
Title : Crystal structure of (3R)-Hydroxyacyl-Acyl Carrier Protein Dehydratase(FabZ) from Helicobacter pylori complexed with compound 1  
Authors : Zhang, L.; Liu, W.; Shen, X.; Jiang, H.  
Deposited on : unknown  
Resolution : 2.42 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

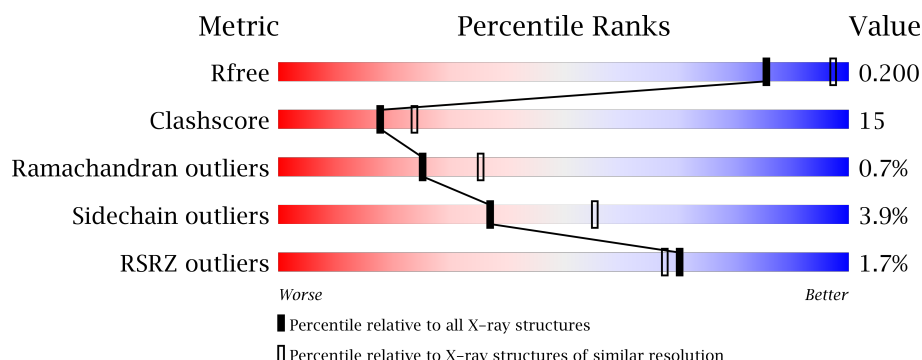
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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))
$R_{free}$	100719	3709 (2.44-2.40)
Clashscore	112137	4241 (2.44-2.40)
Ramachandran outliers	110173	4178 (2.44-2.40)
Sidechain outliers	110143	4179 (2.44-2.40)
RSRZ outliers	101464	3740 (2.44-2.40)

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	171	<div> <div>0.1%</div> <div>64%</div> <div>22%</div> <div>•</div> <div>11%</div> </div>
1	B	171	<div> <div>2%</div> <div>59%</div> <div>28%</div> <div>•</div> <div>12%</div> </div>
1	C	171	<div> <div>0.1%</div> <div>65%</div> <div>23%</div> <div>12%</div> </div>
1	D	171	<div> <div>3%</div> <div>61%</div> <div>25%</div> <div>•</div> <div>11%</div> </div>
1	E	171	<div> <div>0.1%</div> <div>61%</div> <div>25%</div> <div>•</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	171	

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
2	CL	B	1002	-	-	X	-
2	CL	F	1006	-	-	-	X
3	BEN	A	2001	-	-	-	X
3	BEN	A	2004	-	-	X	X
3	BEN	A	2005	-	-	-	X
3	BEN	A	2007	-	-	-	X
3	BEN	A	2009	-	-	-	X
3	BEN	B	2006	-	-	-	X
3	BEN	B	2008	-	-	-	X
3	BEN	C	2010	-	-	-	X
3	BEN	F	2002	-	-	X	X
3	BEN	F	2003	-	-	-	X
4	BDE	C	3002	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7966 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
			1225	803	203	214	5			
1	B	151	Total	C	N	O	S	0	0	0
			1217	797	202	213	5			
1	C	151	Total	C	N	O	S	0	0	0
			1217	797	202	213	5			
1	D	152	Total	C	N	O	S	0	0	0
			1225	803	203	214	5			
1	E	152	Total	C	N	O	S	0	0	0
			1225	803	203	214	5			
1	F	147	Total	C	N	O	S	0	0	0
			1181	778	194	204	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q5G940
A	-10	ARG	-	EXPRESSION TAG	UNP Q5G940
A	-9	GLY	-	EXPRESSION TAG	UNP Q5G940
A	-8	SER	-	EXPRESSION TAG	UNP Q5G940
A	-7	HIS	-	EXPRESSION TAG	UNP Q5G940
A	-6	HIS	-	EXPRESSION TAG	UNP Q5G940
A	-5	HIS	-	EXPRESSION TAG	UNP Q5G940
A	-4	HIS	-	EXPRESSION TAG	UNP Q5G940
A	-3	HIS	-	EXPRESSION TAG	UNP Q5G940
A	-2	HIS	-	EXPRESSION TAG	UNP Q5G940
A	-1	GLY	-	EXPRESSION TAG	UNP Q5G940
A	0	SER	-	EXPRESSION TAG	UNP Q5G940
B	-11	MET	-	EXPRESSION TAG	UNP Q5G940
B	-10	ARG	-	EXPRESSION TAG	UNP Q5G940
B	-9	GLY	-	EXPRESSION TAG	UNP Q5G940
B	-8	SER	-	EXPRESSION TAG	UNP Q5G940
B	-7	HIS	-	EXPRESSION TAG	UNP Q5G940

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	EXPRESSION TAG	UNP Q5G940
B	-5	HIS	-	EXPRESSION TAG	UNP Q5G940
B	-4	HIS	-	EXPRESSION TAG	UNP Q5G940
B	-3	HIS	-	EXPRESSION TAG	UNP Q5G940
B	-2	HIS	-	EXPRESSION TAG	UNP Q5G940
B	-1	GLY	-	EXPRESSION TAG	UNP Q5G940
B	0	SER	-	EXPRESSION TAG	UNP Q5G940
C	-11	MET	-	EXPRESSION TAG	UNP Q5G940
C	-10	ARG	-	EXPRESSION TAG	UNP Q5G940
C	-9	GLY	-	EXPRESSION TAG	UNP Q5G940
C	-8	SER	-	EXPRESSION TAG	UNP Q5G940
C	-7	HIS	-	EXPRESSION TAG	UNP Q5G940
C	-6	HIS	-	EXPRESSION TAG	UNP Q5G940
C	-5	HIS	-	EXPRESSION TAG	UNP Q5G940
C	-4	HIS	-	EXPRESSION TAG	UNP Q5G940
C	-3	HIS	-	EXPRESSION TAG	UNP Q5G940
C	-2	HIS	-	EXPRESSION TAG	UNP Q5G940
C	-1	GLY	-	EXPRESSION TAG	UNP Q5G940
C	0	SER	-	EXPRESSION TAG	UNP Q5G940
D	-11	MET	-	EXPRESSION TAG	UNP Q5G940
D	-10	ARG	-	EXPRESSION TAG	UNP Q5G940
D	-9	GLY	-	EXPRESSION TAG	UNP Q5G940
D	-8	SER	-	EXPRESSION TAG	UNP Q5G940
D	-7	HIS	-	EXPRESSION TAG	UNP Q5G940
D	-6	HIS	-	EXPRESSION TAG	UNP Q5G940
D	-5	HIS	-	EXPRESSION TAG	UNP Q5G940
D	-4	HIS	-	EXPRESSION TAG	UNP Q5G940
D	-3	HIS	-	EXPRESSION TAG	UNP Q5G940
D	-2	HIS	-	EXPRESSION TAG	UNP Q5G940
D	-1	GLY	-	EXPRESSION TAG	UNP Q5G940
D	0	SER	-	EXPRESSION TAG	UNP Q5G940
E	-11	MET	-	EXPRESSION TAG	UNP Q5G940
E	-10	ARG	-	EXPRESSION TAG	UNP Q5G940
E	-9	GLY	-	EXPRESSION TAG	UNP Q5G940
E	-8	SER	-	EXPRESSION TAG	UNP Q5G940
E	-7	HIS	-	EXPRESSION TAG	UNP Q5G940
E	-6	HIS	-	EXPRESSION TAG	UNP Q5G940
E	-5	HIS	-	EXPRESSION TAG	UNP Q5G940
E	-4	HIS	-	EXPRESSION TAG	UNP Q5G940
E	-3	HIS	-	EXPRESSION TAG	UNP Q5G940
E	-2	HIS	-	EXPRESSION TAG	UNP Q5G940
E	-1	GLY	-	EXPRESSION TAG	UNP Q5G940

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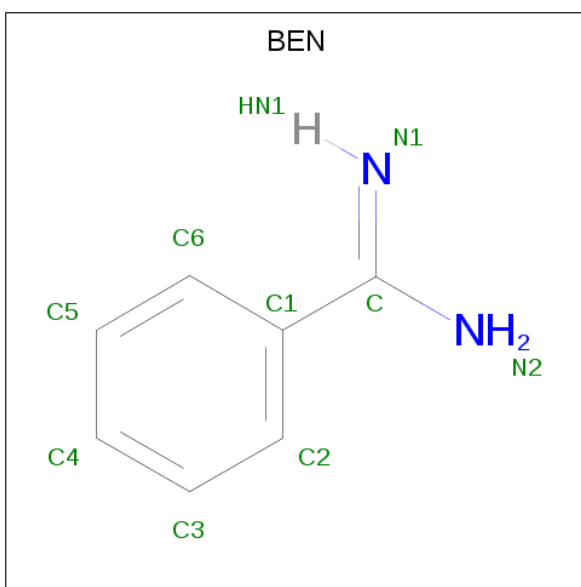
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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	SER	-	EXPRESSION TAG	UNP Q5G940
F	-11	MET	-	EXPRESSION TAG	UNP Q5G940
F	-10	ARG	-	EXPRESSION TAG	UNP Q5G940
F	-9	GLY	-	EXPRESSION TAG	UNP Q5G940
F	-8	SER	-	EXPRESSION TAG	UNP Q5G940
F	-7	HIS	-	EXPRESSION TAG	UNP Q5G940
F	-6	HIS	-	EXPRESSION TAG	UNP Q5G940
F	-5	HIS	-	EXPRESSION TAG	UNP Q5G940
F	-4	HIS	-	EXPRESSION TAG	UNP Q5G940
F	-3	HIS	-	EXPRESSION TAG	UNP Q5G940
F	-2	HIS	-	EXPRESSION TAG	UNP Q5G940
F	-1	GLY	-	EXPRESSION TAG	UNP Q5G940
F	0	SER	-	EXPRESSION TAG	UNP Q5G940

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

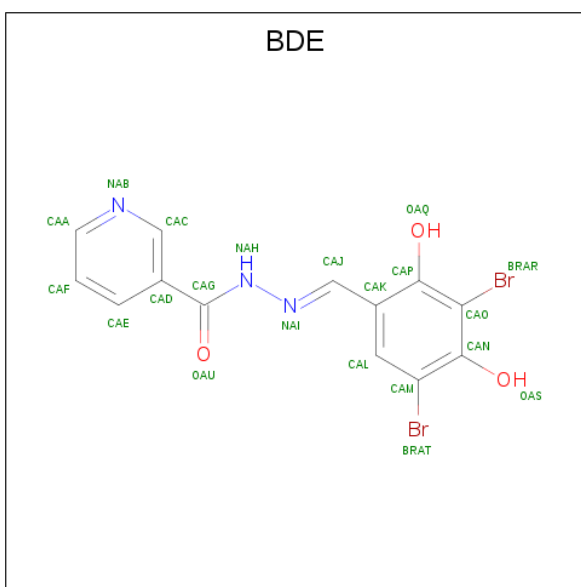
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0

- 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	A	1	Total	C	N	0	0
			9	7	2		
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	F	1	Total	C	N	0	0
			9	7	2		
3	F	1	Total	C	N	0	0
			9	7	2		

- Molecule 4 is N'-[(1E)-(3,5-DIBROMO-2,4-DIHYDROXYPHENYL)METHYLENE]NICOTINOHYDRAZIDE (three-letter code: BDE) (formula: C<sub>13</sub>H<sub>9</sub>Br<sub>2</sub>N<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	Br	C	N	O	0	0
			21	2	13	3	3		
4	C	1	Total	Br	C	N	O	0	0
			21	2	13	3	3		

- Molecule 5 is water.

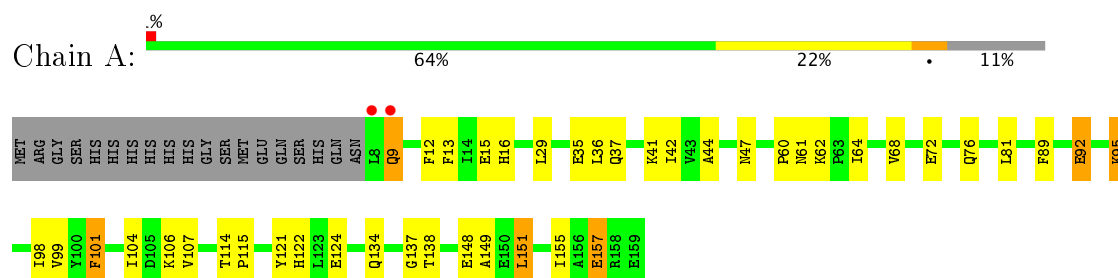
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	105	Total	O	0	0
			105	105		
5	B	92	Total	O	0	0
			92	92		
5	C	76	Total	O	0	0
			76	76		
5	D	80	Total	O	0	0
			80	80		
5	E	101	Total	O	0	0
			101	101		
5	F	84	Total	O	0	0
			84	84		



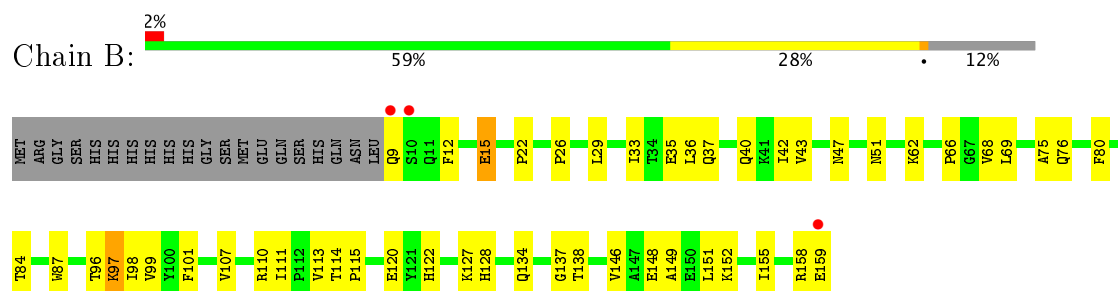
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

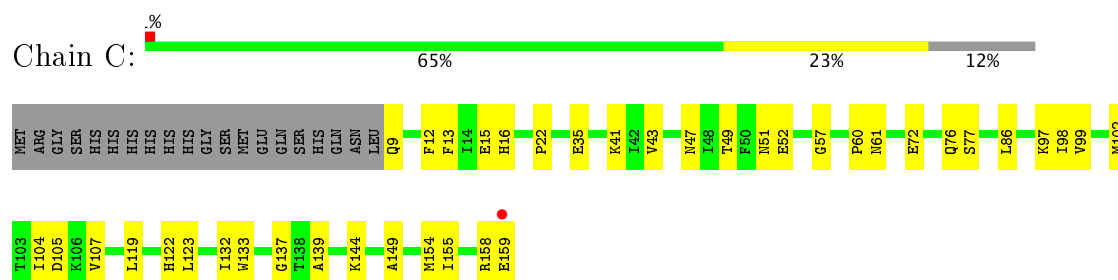
- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase



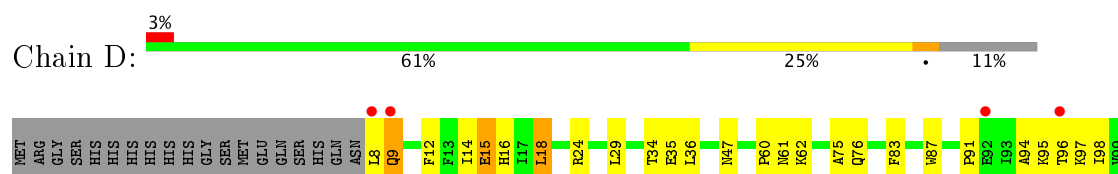
- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase

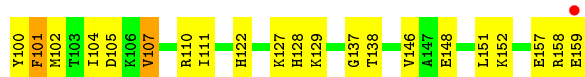


- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase

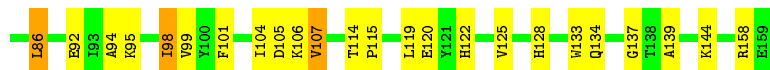
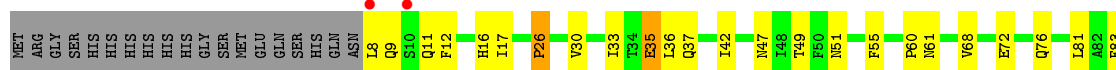


- Molecule 1: (3R)-hydroxymyristoyl-acyl carrier protein dehydratase





- 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, $\alpha$ , $\beta$ , $\gamma$	74.00Å 100.58Å 186.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.42 36.72 – 2.42	Depositor EDS
% Data completeness (in resolution range)	87.4 (50.00-2.42) 92.2 (36.72-2.42)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.39 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.189 , 0.235 0.196 , 0.200	Depositor DCC
$R_{free}$ test set	2540 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.2	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7966	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	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 28.99 % 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 1.6743e-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, 0.333 respectively for untwinned datasets, and 0.375, 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: BDE, 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	0/1256	0.63	0/1698
1	B	0.41	0/1248	0.60	0/1687
1	C	0.41	0/1248	0.62	0/1687
1	D	0.42	0/1256	0.62	0/1698
1	E	0.41	0/1256	0.65	0/1698
1	F	0.41	0/1212	0.63	0/1641
All	All	0.41	0/7476	0.63	0/10109

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	1225	0	1243	44	0
1	B	1217	0	1232	44	0
1	C	1217	0	1232	34	0
1	D	1225	0	1243	44	0
1	E	1225	0	1243	43	0
1	F	1181	0	1200	30	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	2	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	45	0	35	8	0
3	B	18	0	14	1	0
3	C	9	0	7	0	0
3	F	18	0	14	7	0
4	A	21	0	7	3	0
4	C	21	0	7	6	0
5	A	105	0	0	9	0
5	B	92	0	0	3	0
5	C	76	0	0	5	0
5	D	80	0	0	7	0
5	E	101	0	0	9	0
5	F	84	0	0	4	0
All	All	7966	0	7477	227	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 15.

All (227) 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:A:3001:BDE:HAJ	4:A:3001:BDE:OAU	1.67	0.94
1:B:127:LYS:HE3	1:B:134:GLN:NE2	1.85	0.91
1:C:22:PRO:HG3	4:C:3002:BDE:OAQ	1.73	0.89
1:C:13:PHE:H	1:C:16:HIS:HD2	1.16	0.87
4:C:3002:BDE:NAI	4:C:3002:BDE:HAE	1.91	0.85
1:D:91:PRO:O	1:D:95:LYS:HG3	1.80	0.82
1:A:15:GLU:HG3	5:D:1077:HOH:O	1.78	0.82
5:B:2093:HOH:O	1:F:15:GLU:HG2	1.79	0.82
1:B:127:LYS:HE3	1:B:134:GLN:HE22	1.45	0.79
1:A:29:LEU:H	1:A:76:GLN:HE22	1.31	0.79
1:D:29:LEU:H	1:D:76:GLN:HE22	1.29	0.78
1:A:98:ILE:HG13	3:A:2004:BEN:N2	2.00	0.77
1:A:106:LYS:HE3	5:A:3087:HOH:O	1.86	0.75
1:C:104:ILE:HB	1:D:107:VAL:HG13	1.70	0.73
1:A:98:ILE:HA	3:A:2004:BEN:H6	1.70	0.73
1:E:11:GLN:HG2	5:E:1100:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LEU:H	1:B:76:GLN:HE22	1.37	0.70
1:E:107:VAL:CG2	1:F:104:ILE:HB	2.23	0.68
1:A:124:GLU:HG3	5:A:3098:HOH:O	1.94	0.67
1:A:99:VAL:H	3:A:2004:BEN:C	2.07	0.67
1:C:97:LYS:O	4:C:3002:BDE:HAF	1.94	0.67
1:D:9:GLN:HB2	1:D:12:PHE:CZ	2.30	0.66
1:B:99:VAL:HG22	1:B:155:ILE:HG12	1.76	0.66
1:A:35:GLU:OE2	1:A:41:LYS:HE3	1.96	0.66
1:E:104:ILE:HB	1:F:107:VAL:HG22	1.80	0.64
1:E:107:VAL:HG22	1:F:104:ILE:HB	1.79	0.64
1:C:47:ASN:HB3	1:E:47:ASN:HB3	1.78	0.64
1:A:13:PHE:H	1:A:16:HIS:HD2	1.46	0.63
1:D:127:LYS:NZ	1:D:129:LYS:HE3	2.13	0.63
1:C:104:ILE:HB	1:D:107:VAL:CG1	2.29	0.62
1:A:15:GLU:CD	1:A:15:GLU:H	2.02	0.62
1:C:15:GLU:HG2	5:E:1099:HOH:O	1.99	0.62
1:C:105:ASP:HB3	5:C:3076:HOH:O	1.99	0.61
4:C:3002:BDE:NAI	4:C:3002:BDE:CAE	2.59	0.61
1:E:122:HIS:HD2	5:E:1082:HOH:O	1.83	0.61
1:C:102:MET:HE1	1:C:154:MET:HB2	1.83	0.61
1:E:134:GLN:CD	5:E:1096:HOH:O	2.40	0.60
1:A:99:VAL:HG22	1:A:155:ILE:HG12	1.83	0.60
1:E:8:LEU:HD12	1:E:8:LEU:C	2.21	0.60
1:C:132:ILE:N	1:C:132:ILE:HD12	2.17	0.60
1:E:17:ILE:HD13	1:E:30:VAL:HG12	1.84	0.59
1:C:13:PHE:H	1:C:16:HIS:CD2	2.08	0.59
1:D:127:LYS:HZ1	1:D:129:LYS:HE3	1.66	0.58
1:D:138:THR:HG22	1:D:148:GLU:HG2	1.84	0.58
1:D:29:LEU:N	1:D:76:GLN:HE22	2.01	0.58
1:E:60:PRO:O	1:E:61:ASN:HB2	2.04	0.58
5:C:3078:HOH:O	1:D:100:TYR:HE2	1.87	0.58
1:A:9:GLN:HG3	5:A:3066:HOH:O	2.04	0.57
1:E:107:VAL:HG22	1:F:104:ILE:H	1.69	0.57
1:A:36:LEU:HD23	1:A:37:GLN:N	2.20	0.57
1:F:13:PHE:HB2	1:F:15:GLU:OE2	2.04	0.57
1:F:128:HIS:HD2	5:F:2075:HOH:O	1.86	0.57
1:C:60:PRO:O	1:C:61:ASN:HB2	2.05	0.57
5:C:3070:HOH:O	1:D:62:LYS:HE2	2.04	0.56
4:A:3001:BDE:OAU	4:A:3001:BDE:CAJ	2.44	0.56
1:B:127:LYS:HE3	1:B:134:GLN:CD	2.26	0.56
1:D:14:ILE:HG13	1:D:18:LEU:CD2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:ARG:O	1:D:159:GLU:C	2.44	0.55
1:A:101:PHE:H	1:A:101:PHE:HD1	1.54	0.55
1:F:26:PRO:HG3	3:F:2002:BEN:HN21	1.70	0.55
1:E:107:VAL:HG22	1:F:104:ILE:N	2.21	0.55
1:E:36:LEU:HD12	1:E:37:GLN:N	2.22	0.54
1:E:35:GLU:HG3	5:E:1072:HOH:O	2.07	0.54
1:D:83:PHE:CZ	1:D:94:ALA:HB2	2.42	0.54
3:F:2002:BEN:H2	5:F:2055:HOH:O	2.08	0.54
1:E:72:GLU:HG3	1:E:76:GLN:HE21	1.71	0.54
1:A:92:GLU:O	1:A:95:LYS:HG2	2.07	0.54
1:E:104:ILE:HB	1:F:107:VAL:CG2	2.37	0.54
1:D:159:GLU:HG3	1:D:159:GLU:OXT	2.08	0.54
1:E:33:ILE:HD12	1:E:42:ILE:HD11	1.90	0.54
1:E:26:PRO:HB2	3:F:2002:BEN:N1	2.23	0.54
1:A:101:PHE:CD1	1:A:101:PHE:N	2.75	0.53
1:B:66:PRO:HB2	1:B:69:LEU:HG	1.91	0.53
1:D:29:LEU:H	1:D:76:GLN:NE2	2.04	0.53
1:A:47:ASN:HB3	1:D:47:ASN:HB3	1.91	0.53
1:B:96:THR:C	1:B:97:LYS:HD2	2.27	0.53
1:A:15:GLU:OE2	1:A:15:GLU:N	2.28	0.53
1:B:9:GLN:HG3	1:B:12:PHE:CZ	2.44	0.53
1:B:113:VAL:CG2	1:B:146:VAL:HG11	2.39	0.53
1:B:36:LEU:HD23	1:B:37:GLN:N	2.24	0.53
1:C:35:GLU:HB2	1:C:43:VAL:HB	1.90	0.52
1:B:111:ILE:HB	1:B:146:VAL:HG22	1.92	0.52
1:E:120:GLU:OE1	1:E:122:HIS:HE1	1.92	0.52
1:E:68:VAL:HB	1:F:68:VAL:HB	1.90	0.52
1:D:107:VAL:HA	1:D:148:GLU:O	2.09	0.52
1:C:12:PHE:HB3	1:C:16:HIS:HB2	1.91	0.52
1:C:104:ILE:O	1:D:107:VAL:HG13	2.10	0.52
1:E:72:GLU:HG3	1:E:76:GLN:NE2	2.25	0.52
1:E:36:LEU:CD1	1:E:81:LEU:HD13	2.41	0.51
1:B:15:GLU:HG2	5:F:2083:HOH:O	2.09	0.51
1:A:42:ILE:HG22	1:A:81:LEU:HD22	1.91	0.51
1:B:47:ASN:HB3	1:F:47:ASN:HB3	1.92	0.51
1:C:98:ILE:HG23	4:C:3002:BDE:CAL	2.40	0.51
1:E:158:ARG:NH1	1:F:60:PRO:O	2.43	0.51
1:D:111:ILE:HB	1:D:146:VAL:HG12	1.93	0.51
1:A:13:PHE:HB2	1:A:15:GLU:OE2	2.11	0.51
1:B:98:ILE:HD12	1:B:99:VAL:H	1.76	0.51
1:B:138:THR:HG22	1:B:148:GLU:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:HIS:O	1:B:137:GLY:HA3	2.10	0.50
1:B:158:ARG:O	1:B:159:GLU:HB2	2.11	0.50
1:B:35:GLU:HB3	1:B:43:VAL:HB	1.94	0.50
3:F:2002:BEN:N1	5:F:2029:HOH:O	2.35	0.50
1:E:105:ASP:HB3	5:E:1094:HOH:O	2.12	0.50
1:E:95:LYS:HB3	5:E:1035:HOH:O	2.10	0.50
1:A:15:GLU:CG	5:D:1077:HOH:O	2.48	0.50
1:E:98:ILE:HG23	1:E:99:VAL:N	2.27	0.49
1:F:69:LEU:HD21	3:F:2002:BEN:H4	1.94	0.49
1:B:66:PRO:HD2	1:B:69:LEU:HD12	1.94	0.49
1:B:75:ALA:HB1	1:B:101:PHE:CE1	2.47	0.49
1:E:92:GLU:HA	1:E:95:LYS:HZ2	1.77	0.49
1:A:157:GLU:HG3	5:A:3011:HOH:O	2.13	0.49
1:C:99:VAL:H	4:C:3002:BDE:CAJ	2.25	0.49
1:B:33:ILE:HD12	1:B:42:ILE:HD11	1.94	0.49
5:A:3091:HOH:O	1:B:68:VAL:HG22	2.12	0.49
1:B:22:PRO:HB3	1:B:158:ARG:NH1	2.27	0.48
1:E:107:VAL:HG21	1:F:104:ILE:HB	1.94	0.48
1:A:104:ILE:HG12	1:A:151:LEU:HD23	1.95	0.48
1:A:98:ILE:HA	3:A:2004:BEN:C6	2.41	0.48
1:D:60:PRO:HG2	5:D:1035:HOH:O	2.13	0.48
1:C:49:THR:HG23	1:C:52:GLU:HG3	1.94	0.48
4:A:3001:BDE:BRAR	1:B:159:GLU:N	3.00	0.48
1:F:12:PHE:HB2	1:F:33:ILE:HB	1.94	0.48
1:B:97:LYS:O	3:B:2006:BEN:H5	2.14	0.48
1:C:77:SER:HB2	1:C:123:LEU:HD13	1.95	0.48
1:F:23:HIS:O	1:F:24:ARG:HD2	2.14	0.48
1:B:134:GLN:HG2	1:B:152:LYS:HG3	1.96	0.47
1:E:125:VAL:HG11	1:E:128:HIS:HD2	1.79	0.47
1:F:122:HIS:C	1:F:123:LEU:HD22	2.34	0.47
1:A:134:GLN:HG3	5:A:3063:HOH:O	2.15	0.47
5:A:3007:HOH:O	2:B:1002:CL:CL	2.57	0.47
1:D:157:GLU:C	1:D:159:GLU:H	2.16	0.47
1:E:83:PHE:CZ	1:E:94:ALA:HB2	2.49	0.47
1:A:107:VAL:HG22	1:A:149:ALA:CB	2.44	0.47
1:C:107:VAL:HB	1:D:104:ILE:HB	1.96	0.47
1:D:15:GLU:HG2	5:D:1081:HOH:O	2.14	0.47
1:F:107:VAL:HA	1:F:148:GLU:O	2.14	0.47
1:A:95:LYS:HB3	1:A:95:LYS:NZ	2.30	0.47
1:A:138:THR:HG22	1:A:148:GLU:HB3	1.97	0.46
1:A:16:HIS:HB3	1:A:89:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:TRP:CH2	1:D:97:LYS:HE3	2.50	0.46
1:B:114:THR:HB	1:B:115:PRO:HD2	1.97	0.46
1:E:107:VAL:HG22	1:F:104:ILE:CB	2.45	0.46
1:C:98:ILE:HD11	5:C:3070:HOH:O	2.15	0.46
1:A:98:ILE:HG13	3:A:2004:BEN:HN22	1.78	0.46
1:B:107:VAL:HG22	1:B:149:ALA:CB	2.46	0.46
1:D:122:HIS:O	1:D:137:GLY:HA3	2.16	0.46
1:D:34:THR:HG21	5:D:1050:HOH:O	2.16	0.46
1:A:99:VAL:HB	3:A:2004:BEN:N1	2.31	0.46
1:B:98:ILE:HD12	1:B:99:VAL:N	2.31	0.46
5:A:3094:HOH:O	2:B:1002:CL:CL	2.58	0.46
1:F:75:ALA:HB2	1:F:101:PHE:CZ	2.51	0.46
1:F:122:HIS:O	1:F:137:GLY:HA3	2.16	0.45
1:C:15:GLU:CG	5:E:1099:HOH:O	2.61	0.45
1:D:75:ALA:HB2	1:D:101:PHE:CZ	2.52	0.45
1:A:36:LEU:C	1:A:36:LEU:HD23	2.36	0.45
1:A:95:LYS:NZ	1:A:95:LYS:CB	2.80	0.45
1:E:12:PHE:HB3	1:E:16:HIS:HB2	1.99	0.45
1:D:12:PHE:HB3	1:D:16:HIS:HB2	1.99	0.45
1:A:122:HIS:O	1:A:137:GLY:HA3	2.17	0.45
1:F:97:LYS:HA	1:F:156:ALA:O	2.15	0.45
1:C:57:GLY:HA2	1:D:24:ARG:HB2	1.97	0.45
5:A:3089:HOH:O	1:D:15:GLU:HG2	2.17	0.45
1:F:141:VAL:HG23	1:F:146:VAL:HG11	1.99	0.45
1:A:104:ILE:HG12	1:A:151:LEU:CD2	2.46	0.44
1:E:119:LEU:HD11	1:E:139:ALA:HB1	1.99	0.44
1:D:14:ILE:HG13	1:D:18:LEU:HD22	1.99	0.44
1:F:37:GLN:HE21	1:F:40:GLN:NE2	2.16	0.44
1:E:158:ARG:HH12	1:F:61:ASN:HB2	1.83	0.44
1:E:92:GLU:HA	1:E:95:LYS:NZ	2.32	0.44
1:C:107:VAL:HG22	1:C:149:ALA:CB	2.46	0.44
1:C:72:GLU:HG3	1:C:76:GLN:NE2	2.33	0.44
1:C:86:LEU:HD21	1:C:133:TRP:HZ2	1.82	0.43
1:C:122:HIS:O	1:C:137:GLY:HA3	2.17	0.43
1:B:37:GLN:OE1	1:B:40:GLN:NE2	2.52	0.43
1:E:98:ILE:HD13	1:E:158:ARG:HG2	2.01	0.43
1:A:72:GLU:OE1	1:A:101:PHE:CZ	2.71	0.43
1:C:99:VAL:HG22	1:C:155:ILE:HD13	1.99	0.43
1:D:110:ARG:NE	1:D:148:GLU:OE2	2.41	0.43
1:D:127:LYS:HZ1	1:D:129:LYS:CE	2.31	0.43
1:C:13:PHE:N	1:C:16:HIS:HD2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:THR:HB	1:A:115:PRO:CD	2.49	0.43
1:A:62:LYS:HD2	1:A:64:ILE:HD11	2.01	0.43
1:A:114:THR:HB	1:A:115:PRO:HD2	2.00	0.43
1:A:12:PHE:CE2	3:A:2001:BEN:H3	2.54	0.43
1:D:128:HIS:HD2	5:D:1055:HOH:O	2.01	0.43
1:D:36:LEU:C	1:D:36:LEU:HD23	2.38	0.43
1:A:68:VAL:HB	1:B:68:VAL:HB	2.01	0.42
1:E:122:HIS:O	1:E:137:GLY:HA3	2.19	0.42
1:D:61:ASN:HB2	5:D:1078:HOH:O	2.20	0.42
1:F:26:PRO:CG	3:F:2002:BEN:HN21	2.32	0.42
1:B:87:TRP:CZ2	1:B:97:LYS:NZ	2.87	0.42
1:B:120:GLU:HG2	1:B:122:HIS:NE2	2.33	0.42
1:C:158:ARG:HG2	1:C:159:GLU:H	1.84	0.42
1:D:151:LEU:HD12	1:D:151:LEU:C	2.40	0.42
1:B:114:THR:HB	1:B:115:PRO:CD	2.50	0.42
1:C:119:LEU:HD11	1:C:139:ALA:HB1	1.99	0.42
1:B:128:HIS:ND1	5:B:2044:HOH:O	2.32	0.42
1:D:14:ILE:O	1:D:18:LEU:HD22	2.20	0.42
1:E:49:THR:O	1:E:55:PHE:HE1	2.03	0.42
1:E:120:GLU:OE1	1:E:122:HIS:CE1	2.72	0.42
1:A:98:ILE:HA	3:A:2004:BEN:HN21	1.85	0.42
1:B:111:ILE:O	1:B:146:VAL:HG13	2.20	0.42
1:B:120:GLU:OE2	1:B:122:HIS:NE2	2.49	0.42
1:B:151:LEU:HD12	1:B:151:LEU:N	2.35	0.42
1:E:144:LYS:HD2	5:E:1032:HOH:O	2.20	0.41
1:E:86:LEU:HD13	1:E:133:TRP:HZ2	1.83	0.41
1:B:36:LEU:C	1:B:36:LEU:HD23	2.40	0.41
1:A:44:ALA:O	1:A:121:TYR:N	2.46	0.41
1:B:107:VAL:HA	1:B:148:GLU:O	2.20	0.41
1:A:60:PRO:O	1:A:61:ASN:HB2	2.21	0.41
1:D:8:LEU:HD21	1:D:36:LEU:HD21	2.03	0.41
1:D:98:ILE:HG23	1:D:158:ARG:HG2	2.02	0.41
1:F:26:PRO:HG3	3:F:2002:BEN:N2	2.34	0.41
1:C:15:GLU:H	1:C:15:GLU:CD	2.23	0.41
1:E:114:THR:HB	1:E:115:PRO:CD	2.50	0.41
1:B:134:GLN:NE2	5:B:2089:HOH:O	2.52	0.41
1:B:80:PHE:O	1:B:84:THR:HG23	2.21	0.41
1:D:158:ARG:O	1:D:159:GLU:OXT	2.39	0.41
1:F:127:LYS:HE2	1:F:127:LYS:HB3	1.79	0.41
1:B:36:LEU:HD11	1:B:84:THR:OG1	2.21	0.40
1:C:98:ILE:CD1	1:C:158:ARG:HA	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:MET:CE	1:D:152:LYS:HE3	2.52	0.40
1:D:96:THR:C	1:D:97:LYS:HG3	2.40	0.40
1:F:141:VAL:CG2	1:F:146:VAL:HG11	2.51	0.40
1:B:110:ARG:HG2	1:B:110:ARG:HH11	1.85	0.40
1:C:9:GLN:N	5:C:3048:HOH:O	2.54	0.40
1:E:83:PHE:C	1:E:83:PHE:CD2	2.95	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	150/171 (88%)	142 (95%)	8 (5%)	0	100	100
1	B	149/171 (87%)	143 (96%)	5 (3%)	1 (1%)	25	35
1	C	149/171 (87%)	141 (95%)	7 (5%)	1 (1%)	25	35
1	D	150/171 (88%)	141 (94%)	8 (5%)	1 (1%)	25	35
1	E	150/171 (88%)	141 (94%)	8 (5%)	1 (1%)	25	35
1	F	145/171 (85%)	138 (95%)	5 (3%)	2 (1%)	13	17
All	All	893/1026 (87%)	846 (95%)	41 (5%)	6 (1%)	25	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	9	GLN
1	E	51	ASN
1	F	95	LYS
1	F	51	ASN
1	B	51	ASN
1	C	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	131/148 (88%)	125 (95%)	6 (5%)	31	48
1	B	130/148 (88%)	126 (97%)	4 (3%)	45	65
1	C	130/148 (88%)	128 (98%)	2 (2%)	70	84
1	D	131/148 (88%)	125 (95%)	6 (5%)	31	48
1	E	131/148 (88%)	123 (94%)	8 (6%)	22	33
1	F	126/148 (85%)	122 (97%)	4 (3%)	44	64
All	All	779/888 (88%)	749 (96%)	30 (4%)	37	55

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	92	GLU
1	A	95	LYS
1	A	101	PHE
1	A	151	LEU
1	A	157	GLU
1	B	15	GLU
1	B	26	PRO
1	B	62	LYS
1	B	97	LYS
1	C	41	LYS
1	C	144	LYS
1	D	15	GLU
1	D	18	LEU
1	D	35	GLU
1	D	101	PHE
1	D	105	ASP
1	D	107	VAL
1	E	9	GLN
1	E	26	PRO
1	E	35	GLU
1	E	86	LEU

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Mol	Chain	Res	Type
1	E	98	ILE
1	E	101	PHE
1	E	106	LYS
1	E	107	VAL
1	F	15	GLU
1	F	86	LEU
1	F	101	PHE
1	F	107	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	37	GLN
1	A	40	GLN
1	A	51	ASN
1	A	76	GLN
1	B	9	GLN
1	B	40	GLN
1	B	47	ASN
1	B	51	ASN
1	B	76	GLN
1	C	16	HIS
1	C	51	ASN
1	D	9	GLN
1	D	11	GLN
1	D	76	GLN
1	D	128	HIS
1	D	134	GLN
1	D	140	GLN
1	E	37	GLN
1	E	61	ASN
1	E	122	HIS
1	E	134	GLN
1	F	11	GLN
1	F	37	GLN
1	F	40	GLN
1	F	51	ASN
1	F	128	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	1.99	3 (33%)	9,11,11	0.59	0
3	BEN	A	2004	-	9,9,9	1.56	2 (22%)	9,11,11	0.61	0
3	BEN	A	2005	-	9,9,9	1.72	3 (33%)	9,11,11	0.61	0
3	BEN	A	2007	-	9,9,9	2.00	4 (44%)	9,11,11	0.55	0
3	BEN	A	2009	-	9,9,9	1.96	4 (44%)	9,11,11	0.55	0
4	BDE	A	3001	-	22,22,22	2.96	3 (13%)	29,30,30	2.17	10 (34%)
3	BEN	B	2006	-	9,9,9	1.96	4 (44%)	9,11,11	0.56	0
3	BEN	B	2008	-	9,9,9	1.93	3 (33%)	9,11,11	0.61	0
3	BEN	C	2010	-	9,9,9	1.83	3 (33%)	9,11,11	0.60	0
4	BDE	C	3002	-	22,22,22	3.00	3 (13%)	29,30,30	1.50	3 (10%)
3	BEN	F	2002	-	9,9,9	1.65	3 (33%)	9,11,11	0.77	1 (11%)
3	BEN	F	2003	-	9,9,9	1.76	3 (33%)	9,11,11	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BEN	A	2001	-	-	0/4/4/4	0/1/1/1
3	BEN	A	2004	-	-	0/4/4/4	0/1/1/1
3	BEN	A	2005	-	-	0/4/4/4	0/1/1/1
3	BEN	A	2007	-	-	0/4/4/4	0/1/1/1
3	BEN	A	2009	-	-	0/4/4/4	0/1/1/1
4	BDE	A	3001	-	-	0/10/10/10	0/2/2/2
3	BEN	B	2006	-	-	0/4/4/4	0/1/1/1
3	BEN	B	2008	-	-	0/4/4/4	0/1/1/1
3	BEN	C	2010	-	-	0/4/4/4	0/1/1/1
4	BDE	C	3002	-	-	0/10/10/10	0/2/2/2
3	BEN	F	2002	-	-	0/4/4/4	0/1/1/1
3	BEN	F	2003	-	-	0/4/4/4	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3002	BDE	NAH-NAI	-12.79	1.23	1.38
4	A	3001	BDE	NAH-NAI	-12.58	1.23	1.38
4	C	3002	BDE	CAK-CAJ	-3.18	1.39	1.45
4	A	3001	BDE	CAK-CAJ	-3.04	1.39	1.45
3	A	2009	BEN	C4-C3	2.00	1.42	1.38
3	A	2004	BEN	C6-C1	2.04	1.42	1.39
3	A	2007	BEN	C1-C	2.05	1.50	1.47
3	F	2002	BEN	C1-C	2.07	1.50	1.47
3	F	2002	BEN	C-N2	2.17	1.38	1.33
3	A	2001	BEN	C-N2	2.17	1.38	1.33
3	C	2010	BEN	C-N2	2.17	1.38	1.33
3	A	2005	BEN	C6-C1	2.27	1.43	1.39
3	B	2008	BEN	C-N2	2.32	1.39	1.33
3	B	2006	BEN	C-N2	2.32	1.39	1.33
3	A	2005	BEN	C1-C	2.32	1.51	1.47
3	B	2006	BEN	C6-C1	2.35	1.43	1.39
3	A	2005	BEN	C2-C1	2.39	1.43	1.39
3	F	2003	BEN	C6-C1	2.40	1.43	1.39
3	A	2007	BEN	C-N2	2.42	1.39	1.33
3	F	2003	BEN	C-N2	2.45	1.39	1.33
3	C	2010	BEN	C6-C1	2.46	1.43	1.39
3	A	2009	BEN	C-N2	2.52	1.39	1.33
3	A	2009	BEN	C2-C1	2.53	1.43	1.39
3	F	2003	BEN	C2-C1	2.56	1.43	1.39
3	A	2004	BEN	C-N2	2.56	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2008	BEN	C2-C1	2.57	1.43	1.39
3	A	2001	BEN	C2-C1	2.58	1.43	1.39
3	A	2009	BEN	C6-C1	2.58	1.43	1.39
3	A	2007	BEN	C6-C1	2.59	1.43	1.39
3	A	2007	BEN	C2-C1	2.64	1.43	1.39
3	B	2008	BEN	C6-C1	2.65	1.43	1.39
3	C	2010	BEN	C2-C1	2.67	1.43	1.39
3	B	2006	BEN	C2-C1	2.69	1.43	1.39
3	F	2002	BEN	C2-C1	2.78	1.43	1.39
3	B	2006	BEN	C1-C	2.87	1.52	1.47
3	A	2001	BEN	C6-C1	2.98	1.44	1.39
4	C	3002	BDE	CAJ-NAI	4.00	1.32	1.28
4	A	3001	BDE	CAJ-NAI	4.28	1.32	1.28

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3001	BDE	CAP-CAK-CAJ	-5.22	115.33	121.06
4	A	3001	BDE	BRAT-CAM-CAN	-2.20	116.28	118.82
4	A	3001	BDE	CAD-CAC-NAB	-2.09	120.26	123.45
3	F	2002	BEN	C1-C-N2	2.05	121.27	118.12
4	A	3001	BDE	CAK-CAP-CAO	2.47	120.52	118.10
4	A	3001	BDE	CAG-NAH-NAI	2.78	123.02	118.94
4	A	3001	BDE	CAJ-NAI-NAH	2.80	120.52	115.91
4	A	3001	BDE	BRAT-CAM-CAL	2.81	123.19	118.39
4	C	3002	BDE	CAK-CAJ-NAI	3.05	125.26	120.69
4	C	3002	BDE	CAA-NAB-CAC	3.28	122.57	116.83
4	A	3001	BDE	CAL-CAK-CAJ	3.39	124.65	119.60
4	A	3001	BDE	CAA-NAB-CAC	3.48	122.93	116.83
4	C	3002	BDE	CAG-NAH-NAI	4.87	126.09	118.94
4	A	3001	BDE	CAK-CAJ-NAI	5.83	129.44	120.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	BEN	1	0
3	A	2004	BEN	7	0
4	A	3001	BDE	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2006	BEN	1	0
4	C	3002	BDE	6	0
3	F	2002	BEN	7	0

## 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	152/171 (88%)	-0.46	2 (1%) 77 75	14, 21, 36, 58	0
1	B	151/171 (88%)	-0.31	3 (1%) 65 62	13, 22, 36, 61	0
1	C	151/171 (88%)	-0.39	1 (0%) 87 86	16, 23, 37, 61	0
1	D	152/171 (88%)	-0.33	5 (3%) 47 44	14, 23, 44, 64	0
1	E	152/171 (88%)	-0.40	2 (1%) 77 75	16, 23, 38, 54	0
1	F	147/171 (85%)	-0.40	2 (1%) 75 73	15, 23, 37, 43	0
All	All	905/1026 (88%)	-0.38	15 (1%) 70 68	13, 23, 39, 64	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	8	LEU	5.1
1	B	159	GLU	4.6
1	A	8	LEU	4.0
1	B	10	SER	4.0
1	B	9	GLN	3.4
1	D	9	GLN	3.4
1	D	8	LEU	2.8
1	E	10	SER	2.6
1	A	9	GLN	2.3
1	F	95	LYS	2.3
1	C	159	GLU	2.2
1	D	96	THR	2.1
1	D	92	GLU	2.1
1	F	96	THR	2.1
1	D	159	GLU	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(Å <sup>2</sup> )	Q<0.9
3	BEN	F	2003	9/9	0.85	0.41	12.24	49,51,53,53	0
3	BEN	A	2004	9/9	0.90	0.33	9.43	43,44,47,47	0
3	BEN	B	2008	9/9	0.86	0.30	8.00	41,42,44,45	0
3	BEN	F	2002	9/9	0.73	0.37	5.85	48,50,53,54	0
3	BEN	A	2007	9/9	0.81	0.21	5.39	33,34,35,35	0
3	BEN	A	2009	9/9	0.78	0.34	5.09	52,53,54,55	0
3	BEN	C	2010	9/9	0.92	0.19	4.46	32,34,39,40	0
2	CL	F	1006	1/1	0.93	0.21	3.72	39,39,39,39	0
4	BDE	C	3002	21/21	0.80	0.31	3.15	57,69,83,91	0
3	BEN	A	2005	9/9	0.93	0.16	2.49	17,19,22,26	0
3	BEN	B	2006	9/9	0.77	0.27	2.09	39,41,44,45	0
3	BEN	A	2001	9/9	0.74	0.36	2.08	45,47,49,49	0
2	CL	E	1005	1/1	0.94	0.19	1.91	43,43,43,43	0
4	BDE	A	3001	21/21	0.75	0.40	1.65	59,67,72,79	0
2	CL	B	1002	1/1	0.97	0.08	-1.48	43,43,43,43	0
2	CL	C	1003	1/1	0.94	0.18	-	40,40,40,40	0
2	CL	A	1001	1/1	0.98	0.10	-	34,34,34,34	0
2	CL	D	1004	1/1	0.85	0.11	-	43,43,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.