



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 10:44 am GMT

PDB ID : 5IE7  
Title : Crystal structure of a lactonase double mutant in complex with substrate b  
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Deposited on : 2016-02-25  
Resolution : 2.50 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 : recalc28906  
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) : recalc28906

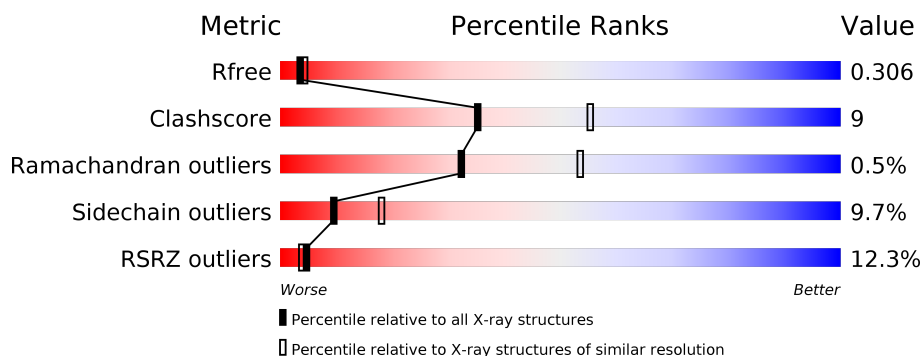
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	264	<div> <div>2%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	B	264	<div> <div>%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	C	264	<div> <div>28%</div> <div>31%</div> <div>14%</div> <div>51%</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5464 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.

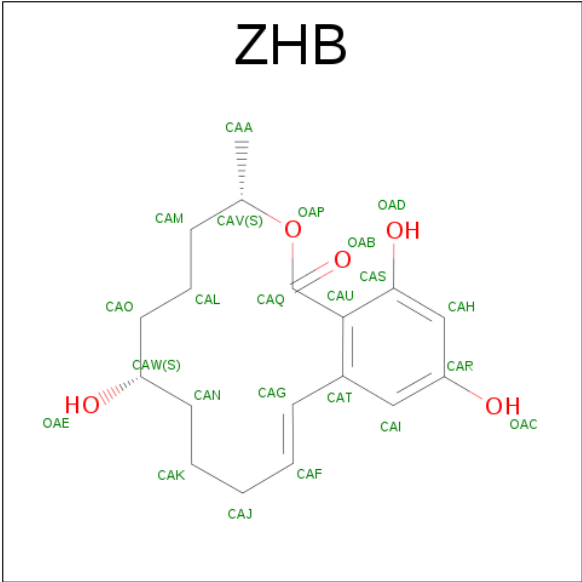
- Molecule 1 is a protein called Zearalenone hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2023	1283	343	386	11			
1	B	264	Total	C	N	O	S	0	0	0
			2023	1283	343	386	11			
1	C	129	Total	C	N	O	S	0	0	0
			988	632	160	191	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	SER	engineered mutation	UNP Q8NKB0
A	153	HIS	VAL	engineered mutation	UNP Q8NKB0
B	102	ALA	SER	engineered mutation	UNP Q8NKB0
B	153	HIS	VAL	engineered mutation	UNP Q8NKB0
C	102	ALA	SER	engineered mutation	UNP Q8NKB0
C	153	HIS	VAL	engineered mutation	UNP Q8NKB0

- Molecule 2 is (3S,7S,11E)-7,14,16-trihydroxy-3-methyl-3,4,5,6,7,8,9,10-octahydro-1H-2-benzoxacyclotetradecin-1-one (three-letter code: ZHB) (formula: C<sub>18</sub>H<sub>24</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	18	5		
2	B	1	Total	C	O	0	0
			23	18	5		

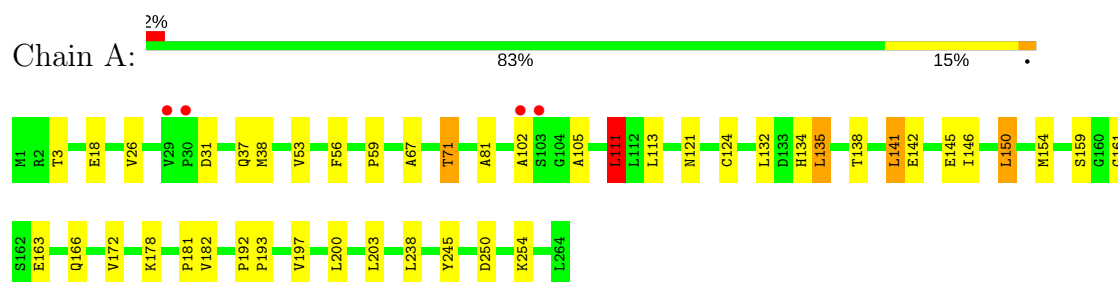
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	153	Total	O	0	0
			153	153		
3	B	119	Total	O	0	0
			119	119		
3	C	112	Total	O	0	0
			112	112		

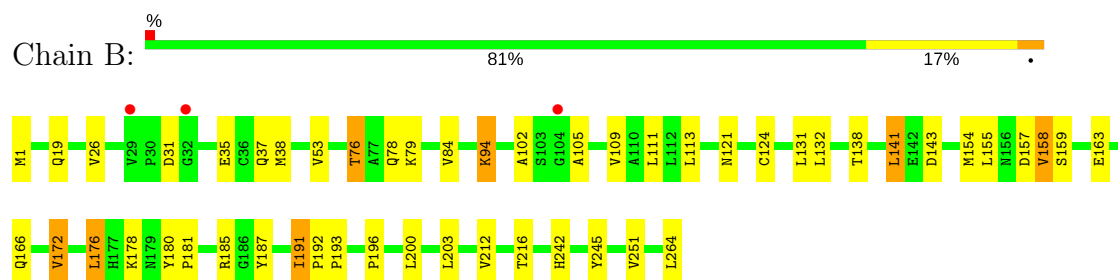
### 3 Residue-property plots

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.

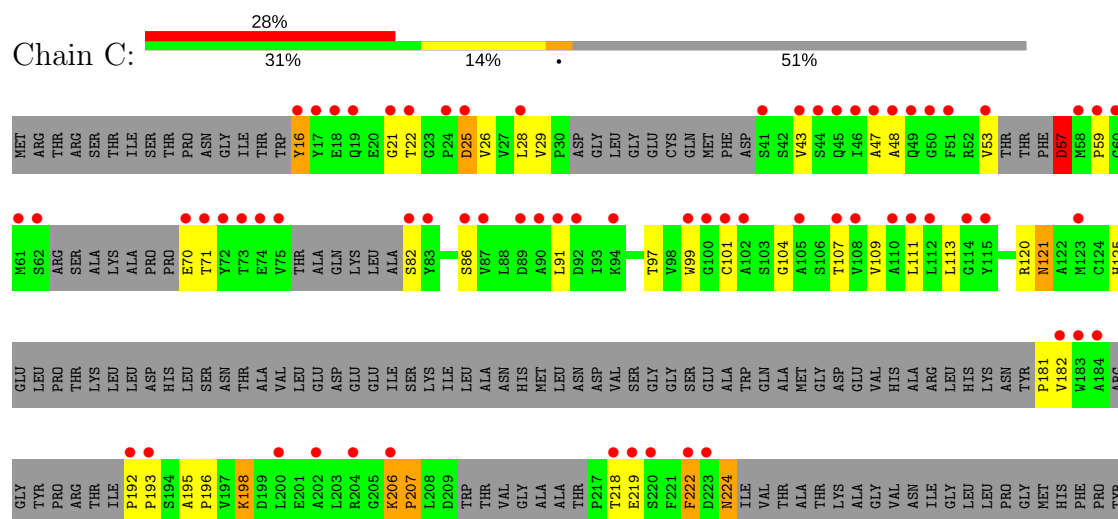
#### • Molecule 1: Zearalenone hydrolase



#### • Molecule 1: Zearalenone hydrolase



#### • Molecule 1: Zearalenone hydrolase



VAL	SER	HIS	PRO
D250			
V251			
F252			
A253			
K254			
Y255			
V256			
V257			
E258			
T259			
T260			
Q261			
K262			
H263			
L264			

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.41 Å 86.41 Å 470.45 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.50 24.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.00-2.50) 99.7 (24.91-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 2.50 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.217 , 0.289 0.239 , 0.306	Depositor DCC
$R_{free}$ test set	1869 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.8	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.5	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	0.92	EDS
Total number of atoms	5464	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: ZHB

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	0.56	0/2075	0.76	1/2834 (0.0%)
1	B	0.54	0/2075	0.75	0/2834
1	C	0.48	0/1006	0.63	0/1361
All	All	0.54	0/5156	0.73	1/7029 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	3
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	LEU	CA-CB-CG	5.96	129.02	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	157	ASP	Peptide
1	C	181	PRO	Peptide
1	C	48	ALA	Peptide
1	C	57	ASP	Peptide



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2023	0	1989	23	0
1	B	2023	0	1989	39	0
1	C	988	0	959	30	0
2	A	23	0	0	1	0
2	B	23	0	0	2	0
3	A	153	0	0	0	0
3	B	119	0	0	4	0
3	C	112	0	0	5	0
All	All	5464	0	4937	93	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 9.

All (93) 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:B:212:VAL:HG13	3:B:411:HOH:O	1.70	0.92
1:B:76:THR:HG22	1:B:79:LYS:H	1.33	0.92
1:A:38:MET:CE	1:A:245:TYR:HE2	1.87	0.88
1:B:38:MET:CE	1:B:245:TYR:HE2	1.85	0.88
1:B:38:MET:HE3	1:B:245:TYR:HE2	1.41	0.84
1:C:16:TYR:O	1:C:57:ASP:HB3	1.77	0.84
1:B:212:VAL:CG1	3:B:411:HOH:O	2.23	0.84
1:B:109:VAL:HG22	1:B:196:PRO:HG2	1.57	0.83
1:A:38:MET:HE3	1:A:245:TYR:HE2	1.41	0.83
1:C:182:VAL:O	1:C:182:VAL:HG13	1.83	0.78
1:A:31:ASP:OD2	1:A:38:MET:HE1	1.82	0.78
1:B:31:ASP:OD2	1:B:38:MET:HE1	1.83	0.77
1:B:76:THR:CG2	1:B:79:LYS:H	2.01	0.73
1:B:38:MET:HE3	1:B:245:TYR:CE2	2.23	0.73
1:A:67:ALA:HB1	1:A:71:THR:HG21	1.69	0.73
1:C:255:TYR:OH	3:C:301:HOH:O	2.06	0.72
1:A:38:MET:HE3	1:A:245:TYR:CE2	2.23	0.71
1:B:172:VAL:HG23	1:B:176:LEU:HD22	1.76	0.68
1:B:76:THR:HG23	1:B:78:GLN:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:HIS:CE1	1:A:135:LEU:HD13	2.33	0.64
1:C:101:CYS:HA	1:C:125:HIS:HB2	1.82	0.62
1:C:57:ASP:N	1:C:57:ASP:OD1	2.34	0.60
1:C:206:LYS:HD3	1:C:207:PRO:HD2	1.88	0.56
1:A:59:PRO:HB2	1:A:71:THR:HG23	1.87	0.56
1:B:109:VAL:HG22	1:B:196:PRO:CG	2.32	0.56
1:C:252:PHE:O	1:C:256:VAL:HG23	2.06	0.56
1:A:38:MET:CE	1:A:245:TYR:CE2	2.79	0.55
1:B:155:LEU:HD13	1:B:166:GLN:HG2	1.87	0.55
1:C:182:VAL:O	1:C:182:VAL:CG1	2.55	0.55
1:B:158:VAL:HG13	1:B:242:HIS:HD2	1.72	0.54
1:C:251:VAL:HG23	3:C:342:HOH:O	2.07	0.53
1:A:81:ALA:HB1	1:A:111:LEU:HD13	1.90	0.52
1:C:222:PHE:C	1:C:222:PHE:CD1	2.83	0.52
1:C:97:THR:HG1	1:C:120:ARG:HE	1.57	0.52
2:B:301:ZHB:OAP	2:B:301:ZHB:CAG	2.56	0.51
1:B:94:LYS:HD3	1:B:94:LYS:H	1.75	0.51
1:B:94:LYS:HD3	1:B:94:LYS:N	2.25	0.51
1:A:102:ALA:HB1	2:A:300:ZHB:CAQ	2.40	0.50
1:B:155:LEU:CD1	1:B:166:GLN:HG2	2.42	0.50
1:C:120:ARG:HD3	3:C:330:HOH:O	2.11	0.50
1:B:38:MET:CE	1:B:245:TYR:CE2	2.78	0.50
1:B:143:ASP:OD1	1:B:185:ARG:NH1	2.38	0.48
1:B:84:VAL:CG2	1:B:111:LEU:HD11	2.43	0.48
1:B:84:VAL:HG21	1:B:111:LEU:HD11	1.95	0.48
1:C:29:VAL:HG11	1:C:107:THR:HG21	1.96	0.48
1:B:109:VAL:CG2	1:B:196:PRO:HG2	2.36	0.48
1:C:224:ASN:HA	3:C:350:HOH:O	2.13	0.47
1:B:154:MET:O	1:B:159:SER:HB3	2.14	0.47
1:C:255:TYR:O	1:C:259:THR:OG1	2.33	0.47
1:A:37:GLN:HG2	1:A:172:VAL:CG2	2.44	0.47
1:C:192:PRO:HB2	1:C:193:PRO:HD3	1.96	0.47
1:C:97:THR:OG1	1:C:260:THR:HG23	2.15	0.46
1:C:120:ARG:HG2	1:C:121:ASN:HD22	1.81	0.46
1:B:138:THR:HA	1:B:141:LEU:HD22	1.98	0.46
1:A:59:PRO:CB	1:A:71:THR:HG23	2.46	0.45
1:B:105:ALA:HB1	1:B:124:CYS:HB2	1.99	0.45
1:B:94:LYS:CD	1:B:94:LYS:N	2.80	0.45
1:A:138:THR:HA	1:A:141:LEU:HD22	1.98	0.45
1:A:134:HIS:ND1	1:A:135:LEU:HD13	2.31	0.44
1:A:154:MET:O	1:A:159:SER:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASP:OD2	1:A:38:MET:CE	2.61	0.44
1:B:158:VAL:HG13	1:B:242:HIS:CD2	2.51	0.44
1:A:250:ASP:OD2	1:A:254:LYS:HE2	2.15	0.44
1:B:76:THR:HG23	1:B:78:GLN:N	2.29	0.44
1:C:195:ALA:O	1:C:198:LYS:HE2	2.18	0.43
1:B:19:GLN:HA	1:B:53:VAL:O	2.18	0.43
1:C:28:LEU:HD22	1:C:252:PHE:HZ	1.83	0.43
1:A:3:THR:O	1:A:18:GLU:HA	2.18	0.43
1:C:26:VAL:O	1:C:53:VAL:HA	2.17	0.43
1:B:180:TYR:N	1:B:181:PRO:CD	2.82	0.43
1:C:21:GLY:CA	1:C:47:ALA:HB1	2.49	0.43
1:B:178:LYS:O	1:B:181:PRO:HD2	2.19	0.43
1:B:26:VAL:O	1:B:53:VAL:HA	2.19	0.43
1:C:192:PRO:HD2	3:C:307:HOH:O	2.18	0.42
1:A:146:ILE:CG2	1:A:150:LEU:HD22	2.49	0.42
1:A:105:ALA:HB1	1:A:124:CYS:HB2	2.01	0.42
1:B:94:LYS:HG2	3:B:413:HOH:O	2.19	0.42
1:C:222:PHE:O	1:C:222:PHE:CD1	2.72	0.42
1:B:35:GLU:OE2	1:B:37:GLN:HB3	2.20	0.42
1:C:70:GLU:O	1:C:71:THR:C	2.58	0.42
1:A:26:VAL:O	1:A:53:VAL:HA	2.19	0.41
1:B:102:ALA:HB1	2:B:301:ZHB:CAQ	2.50	0.41
1:B:180:TYR:HB2	1:B:181:PRO:HD3	2.02	0.41
1:C:104:GLY:O	1:C:107:THR:HB	2.21	0.41
1:B:187:TYR:CD2	1:B:191:ILE:HD13	2.54	0.41
1:C:109:VAL:CG1	1:C:196:PRO:HG2	2.50	0.41
1:A:178:LYS:O	1:A:181:PRO:HD2	2.20	0.41
1:C:25:ASP:O	1:C:120:ARG:NH2	2.54	0.41
1:B:192:PRO:HB2	1:B:193:PRO:HD3	2.02	0.41
1:C:59:PRO:HB2	1:C:71:THR:CG2	2.50	0.41
1:A:192:PRO:HB2	1:A:193:PRO:HD3	2.02	0.41
1:B:216:THR:HB	3:B:411:HOH:O	2.20	0.40
1:C:70:GLU:O	1:C:70:GLU:HG2	2.20	0.40

There are no symmetry-related clashes.

## 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	262/264 (99%)	247 (94%)	14 (5%)	1 (0%)	38	59
1	B	262/264 (99%)	249 (95%)	13 (5%)	0	100	100
1	C	111/264 (42%)	98 (88%)	11 (10%)	2 (2%)	10	17
All	All	635/792 (80%)	594 (94%)	38 (6%)	3 (0%)	32	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	207	PRO
1	A	161	GLY
1	C	43	VAL

### 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	220/220 (100%)	202 (92%)	18 (8%)	13	25
1	B	220/220 (100%)	203 (92%)	17 (8%)	15	28
1	C	109/220 (50%)	91 (84%)	18 (16%)	2	4
All	All	549/660 (83%)	496 (90%)	53 (10%)	9	18

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	PHE
1	A	71	THR
1	A	111	LEU
1	A	113	LEU
1	A	121	ASN
1	A	132	LEU
1	A	135	LEU
1	A	141	LEU
1	A	142	GLU
1	A	145	GLU
1	A	150	LEU
1	A	163	GLU
1	A	166	GLN
1	A	182	VAL
1	A	197	VAL
1	A	200	LEU
1	A	203	LEU
1	A	238	LEU
1	B	1	MET
1	B	76	THR
1	B	94	LYS
1	B	113	LEU
1	B	121	ASN
1	B	131	LEU
1	B	132	LEU
1	B	141	LEU
1	B	158	VAL
1	B	163	GLU
1	B	172	VAL
1	B	176	LEU
1	B	191	ILE
1	B	200	LEU
1	B	203	LEU
1	B	251	VAL
1	B	264	LEU
1	C	16	TYR
1	C	22	THR
1	C	25	ASP
1	C	57	ASP
1	C	82	SER
1	C	86	SER
1	C	91	LEU
1	C	99	TRP

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Mol	Chain	Res	Type
1	C	111	LEU
1	C	113	LEU
1	C	121	ASN
1	C	198	LYS
1	C	206	LYS
1	C	218	THR
1	C	219	GLU
1	C	222	PHE
1	C	224	ASN
1	C	259	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	121	ASN
1	A	156	ASN
1	A	166	GLN
1	A	177	HIS
1	B	121	ASN
1	B	137	ASN
1	B	177	HIS
1	B	261	GLN
1	C	121	ASN
1	C	125	HIS
1	C	224	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

2 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	ZHB	A	300	-	24,24,24	1.46	4 (16%)	32,32,32	1.62	6 (18%)
2	ZHB	B	301	-	24,24,24	1.43	3 (12%)	32,32,32	1.30	5 (15%)

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	ZHB	A	300	-	-	0/22/22/22	0/1/2/2
2	ZHB	B	301	-	-	0/22/22/22	0/1/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	ZHB	CAT-CAG	-4.50	1.40	1.47
2	B	301	ZHB	CAT-CAG	-4.09	1.41	1.47
2	A	300	ZHB	CAU-CAQ	-3.93	1.40	1.50
2	B	301	ZHB	CAU-CAQ	-3.86	1.41	1.50
2	A	300	ZHB	CAJ-CAF	-2.25	1.38	1.50
2	B	301	ZHB	CAG-CAF	2.46	1.39	1.31
2	A	300	ZHB	CAG-CAF	2.47	1.39	1.31

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	ZHB	CAK-CAN-CAW	-3.86	103.47	115.00
2	A	300	ZHB	CAT-CAG-CAF	-3.81	117.29	125.52
2	A	300	ZHB	CAA-CAV-CAM	-3.41	104.42	113.99
2	A	300	ZHB	CAL-CAO-CAW	-3.06	105.86	115.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ZHB	CAJ-CAF-CAG	-2.71	120.14	125.50
2	A	300	ZHB	CAI-CAT-CAG	-2.39	115.27	120.70
2	B	301	ZHB	CAK-CAN-CAW	-2.37	107.93	115.00
2	B	301	ZHB	CAA-CAV-CAM	-2.16	107.92	113.99
2	A	300	ZHB	CAN-CAK-CAJ	-2.11	109.96	114.37
2	B	301	ZHB	OAP-CAV-CAA	2.15	112.94	107.95
2	B	301	ZHB	CAV-OAP-CAQ	3.50	124.15	117.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	ZHB	1	0
2	B	301	ZHB	2	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	264/264 (100%)	-0.24	4 (1%) 74 75	15, 23, 42, 62	0
1	B	264/264 (100%)	-0.10	3 (1%) 80 81	17, 26, 43, 68	0
1	C	129/264 (48%)	2.60	74 (57%) 0 0	49, 70, 90, 102	0
All	All	657/792 (82%)	0.37	81 (12%) 5 4	15, 26, 79, 102	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	24	PRO	9.7
1	C	46	ILE	7.8
1	C	72	TYR	7.5
1	C	193	PRO	6.8
1	C	60	GLY	6.6
1	C	28	LEU	6.5
1	C	90	ALA	6.4
1	C	219	GLU	6.2
1	C	222	PHE	6.0
1	C	18	GLU	6.0
1	C	47	ALA	5.8
1	C	75	VAL	5.5
1	C	61	MET	5.3
1	C	89	ASP	5.2
1	C	73	THR	5.2
1	C	202	ALA	5.1
1	C	62	SER	5.1
1	C	182	VAL	4.9
1	C	111	LEU	4.7
1	C	41	SER	4.7
1	C	223	ASP	4.6
1	C	183	TRP	4.6
1	C	184	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	110	ALA	4.5
1	C	259	THR	4.3
1	C	71	THR	4.2
1	C	218	THR	4.1
1	C	220	SER	4.0
1	C	87	VAL	4.0
1	C	83	TYR	4.0
1	C	51	PHE	3.9
1	C	43	VAL	3.9
1	C	115	TYR	3.8
1	C	114	GLY	3.7
1	C	44	SER	3.7
1	C	200	LEU	3.6
1	C	49	GLN	3.6
1	C	108	VAL	3.5
1	C	251	VAL	3.5
1	C	19	GLN	3.4
1	C	16	TYR	3.3
1	C	123	MET	3.3
1	C	45	GLN	3.3
1	C	86	SER	3.2
1	C	59	PRO	3.2
1	A	29	VAL	3.1
1	C	112	LEU	3.0
1	C	70	GLU	3.0
1	C	101	CYS	2.9
1	C	107	THR	2.8
1	C	25	ASP	2.8
1	A	102	ALA	2.8
1	C	105	ALA	2.8
1	C	17	TYR	2.7
1	C	192	PRO	2.7
1	B	104	GLY	2.7
1	C	50	GLY	2.5
1	C	92	ASP	2.5
1	A	103	SER	2.5
1	C	102	ALA	2.5
1	C	91	LEU	2.5
1	C	82	SER	2.4
1	A	30	PRO	2.4
1	B	29	VAL	2.4
1	C	48	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	253	ALA	2.3
1	C	204	ARG	2.3
1	C	21	GLY	2.3
1	C	74	GLU	2.3
1	C	262	LYS	2.2
1	C	53	VAL	2.2
1	C	258	GLU	2.2
1	C	99	TRP	2.2
1	C	255	TYR	2.2
1	C	22	THR	2.2
1	C	94	LYS	2.2
1	C	252	PHE	2.1
1	C	100	GLY	2.1
1	B	32	GLY	2.1
1	C	206	LYS	2.0
1	C	58	MET	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
2	ZHB	A	300	23/23	0.93	0.30	1.89	29,42,52,54	0
2	ZHB	B	301	23/23	0.94	0.27	1.68	30,39,54,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.