



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:42 am BST

PDB ID : 4N44  
Title : Crystal structure of oxidized form of thiolase from *Clostridium acetobutylicum*  
Authors : Kim, S.; Ha, S.C.; Ahn, J.W.; Kim, E.J.; Lim, J.H.; Kim, K.J.  
Deposited on : 2013-10-08  
Resolution : 1.77 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 : 2.11  
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) : 2.11

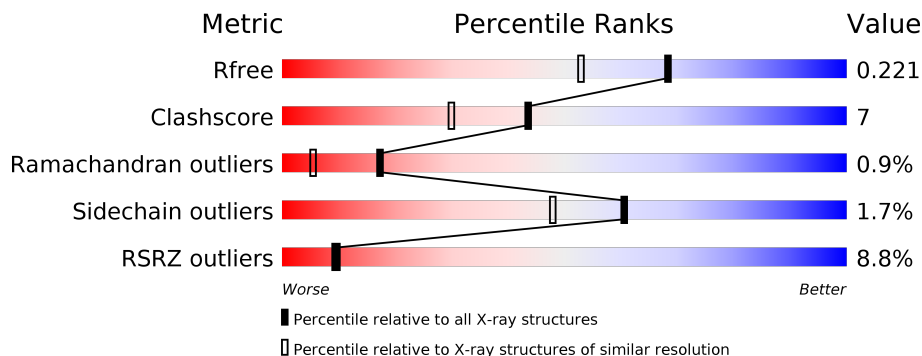
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.77 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	400	
1	B	400	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6249 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 Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	392	2892	1824	501	552	15	0	0	0
1	B	392	2892	1824	501	552	15	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	393	LEU	-	EXPRESSION TAG	UNP F0K5D8
A	394	GLU	-	EXPRESSION TAG	UNP F0K5D8
A	395	HIS	-	EXPRESSION TAG	UNP F0K5D8
A	396	HIS	-	EXPRESSION TAG	UNP F0K5D8
A	397	HIS	-	EXPRESSION TAG	UNP F0K5D8
A	398	HIS	-	EXPRESSION TAG	UNP F0K5D8
A	399	HIS	-	EXPRESSION TAG	UNP F0K5D8
A	400	HIS	-	EXPRESSION TAG	UNP F0K5D8
B	393	LEU	-	EXPRESSION TAG	UNP F0K5D8
B	394	GLU	-	EXPRESSION TAG	UNP F0K5D8
B	395	HIS	-	EXPRESSION TAG	UNP F0K5D8
B	396	HIS	-	EXPRESSION TAG	UNP F0K5D8
B	397	HIS	-	EXPRESSION TAG	UNP F0K5D8
B	398	HIS	-	EXPRESSION TAG	UNP F0K5D8
B	399	HIS	-	EXPRESSION TAG	UNP F0K5D8
B	400	HIS	-	EXPRESSION TAG	UNP F0K5D8

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

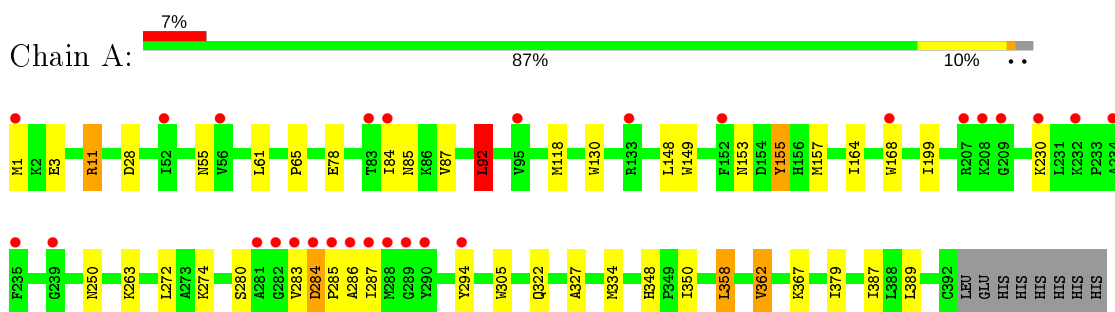
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	225	Total	O	0	0
			225	225		
4	B	212	Total	O	0	0
			212	212		

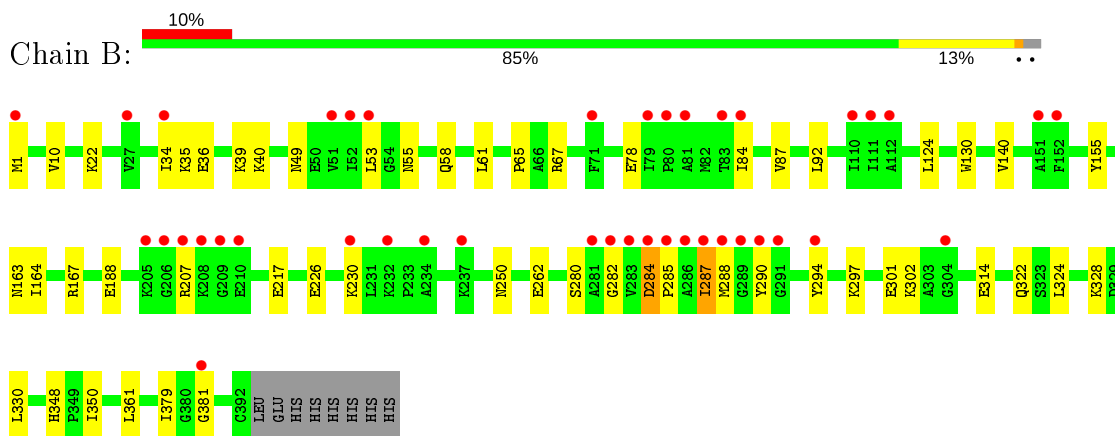
### 3 Residue-property plots [i](#)

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



- Molecule 1: Acetyl-CoA acetyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.23Å 53.99Å 72.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.44 – 1.77 43.40 – 1.77	Depositor EDS
% Data completeness (in resolution range)	98.5 (43.44-1.77) 98.5 (43.40-1.77)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 1.77Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.168 , 0.208 0.183 , 0.221	Depositor DCC
$R_{free}$ test set	3911 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtrriage
Anisotropy	0.669	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6249	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.12	7/2933 (0.2%)	1.02	6/3958 (0.2%)
1	B	1.11	3/2933 (0.1%)	1.02	2/3958 (0.1%)
All	All	1.12	10/5866 (0.2%)	1.02	8/7916 (0.1%)

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	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	TRP	CD2-CE2	6.86	1.49	1.41
1	A	305	TRP	CD2-CE2	5.83	1.48	1.41
1	A	65	PRO	N-CD	5.72	1.55	1.47
1	B	65	PRO	N-CD	5.64	1.55	1.47
1	B	130	TRP	CG-CD1	5.51	1.44	1.36
1	A	362	VAL	CB-CG2	-5.43	1.41	1.52
1	A	130	TRP	CG-CD1	5.40	1.44	1.36
1	A	168	TRP	CD2-CE2	5.40	1.47	1.41
1	A	149	TRP	CD2-CE2	5.37	1.47	1.41
1	B	285	PRO	N-CD	5.36	1.55	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	LEU	CB-CG-CD2	6.65	122.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	LYS	CD-CE-NZ	-6.33	97.15	111.70
1	A	118	MET	CG-SD-CE	5.75	109.40	100.20
1	A	28	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	67	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	358	LEU	CB-CG-CD1	-5.32	101.96	111.00
1	B	67	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	11	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	207	ARG	Peptide
1	B	284	ASP	Peptide

## 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	2892	0	2961	47	0
1	B	2892	0	2961	39	0
2	A	8	0	6	0	0
2	B	8	0	6	0	0
3	B	12	0	16	3	0
4	A	225	0	0	7	0
4	B	212	0	0	8	0
All	All	6249	0	5950	79	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 7.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ALA:HB1	1:A:334:MET:CE	1.68	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:GLU:OE2	1:B:40:LYS:HE3	1.55	1.06
1:A:230:LYS:HE3	4:A:627:HOH:O	1.58	1.04
1:A:327:ALA:HB1	1:A:334:MET:HE1	1.06	1.03
1:B:217:GLU:O	3:B:403:GOL:H11	1.63	0.99
1:A:294:TYR:OH	1:B:78:GLU:HB2	1.75	0.86
1:A:274:LYS:HE2	4:A:719:HOH:O	1.75	0.85
1:A:327:ALA:CB	1:A:334:MET:CE	2.55	0.81
1:A:362:VAL:HG12	1:A:389:LEU:CD1	2.13	0.78
3:B:403:GOL:H12	4:B:703:HOH:O	1.86	0.74
1:A:283:VAL:HG22	1:A:284:ASP:H	1.53	0.73
1:A:327:ALA:CB	1:A:334:MET:HE1	2.02	0.73
1:A:84:ILE:HD12	1:B:84:ILE:HD12	1.75	0.69
1:B:188:GLU:CG	4:B:628:HOH:O	2.40	0.69
1:B:40:LYS:HD3	4:B:609:HOH:O	1.93	0.67
1:A:287:ILE:HG13	1:A:294:TYR:CD2	2.30	0.67
1:A:367:LYS:HE2	4:A:606:HOH:O	1.95	0.65
1:A:327:ALA:HB1	1:A:334:MET:HE3	1.74	0.65
1:A:164:ILE:HD11	1:A:379:ILE:CD1	2.28	0.63
1:B:188:GLU:HG2	4:B:628:HOH:O	2.00	0.60
1:A:287:ILE:HG13	1:A:294:TYR:HD2	1.66	0.59
1:B:40:LYS:CD	4:B:609:HOH:O	2.49	0.59
1:A:327:ALA:CB	1:A:334:MET:HE3	2.33	0.58
1:A:280:SER:HB3	4:B:517:HOH:O	2.05	0.57
1:B:250:ASN:HD22	1:B:348:HIS:H	1.51	0.57
1:A:362:VAL:HG12	1:A:389:LEU:HD13	1.86	0.56
1:B:282:GLY:HA3	1:B:302:LYS:NZ	2.21	0.56
1:B:324:LEU:O	1:B:328:LYS:HG3	2.06	0.56
1:B:188:GLU:CB	4:B:628:HOH:O	2.54	0.56
1:A:84:ILE:HD12	1:B:84:ILE:CD1	2.36	0.55
1:A:92:LEU:HD22	1:A:387:ILE:HD12	1.89	0.54
1:B:282:GLY:HA3	1:B:302:LYS:HZ2	1.71	0.54
1:B:297:LYS:HE2	1:B:330:LEU:CD2	2.38	0.54
1:A:294:TYR:HH	1:B:78:GLU:HB2	1.71	0.53
1:A:250:ASN:HD22	1:A:348:HIS:H	1.56	0.53
1:B:250:ASN:ND2	1:B:348:HIS:H	2.07	0.53
1:A:164:ILE:HD11	1:A:379:ILE:HD11	1.91	0.53
1:B:188:GLU:HB3	4:B:628:HOH:O	2.09	0.53
1:B:163:ASN:O	1:B:167:ARG:HG3	2.09	0.53
1:A:148:LEU:O	1:A:157:MET:HG2	2.09	0.53
1:B:290:TYR:OH	1:B:301:GLU:OE1	2.20	0.52
1:A:283:VAL:HG22	1:A:284:ASP:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:N	1:A:272:LEU:HD12	2.24	0.52
1:A:283:VAL:HG23	1:B:49:ASN:ND2	2.24	0.51
4:A:569:HOH:O	1:B:280:SER:HB3	2.09	0.51
1:A:283:VAL:CG2	1:A:284:ASP:H	2.23	0.51
1:A:78:GLU:HB2	1:B:294:TYR:OH	2.11	0.51
1:A:250:ASN:ND2	1:A:348:HIS:H	2.09	0.50
1:B:290:TYR:HB3	1:B:297:LYS:HD2	1.92	0.50
1:A:358:LEU:O	1:A:362:VAL:HG13	2.11	0.50
1:A:272:LEU:N	1:A:272:LEU:CD1	2.75	0.49
1:A:164:ILE:HD13	1:A:322:GLN:HG2	1.95	0.49
1:A:55:ASN:HD21	1:A:61:LEU:HD12	1.78	0.49
1:A:85:ASN:HD22	1:B:58:GLN:NE2	2.11	0.48
1:A:367:LYS:CE	4:A:606:HOH:O	2.59	0.47
1:B:217:GLU:O	3:B:403:GOL:C1	2.50	0.47
1:B:10:VAL:CG2	1:B:40:LYS:HD2	2.45	0.46
1:A:164:ILE:CD1	1:A:379:ILE:HD13	2.47	0.45
1:A:153:ASN:HB3	1:A:155:TYR:CE2	2.52	0.45
1:A:78:GLU:HG3	1:B:287:ILE:HG21	1.99	0.45
1:A:92:LEU:HD22	1:A:387:ILE:CD1	2.47	0.44
1:B:226:GLU:O	1:B:230:LYS:HG3	2.18	0.44
1:B:34:ILE:HD11	1:B:53:LEU:HD11	2.00	0.44
1:B:35:LYS:NZ	1:B:39:LYS:NZ	2.66	0.43
1:A:230:LYS:CE	4:A:627:HOH:O	2.35	0.43
1:A:285:PRO:HA	1:A:286:ALA:HA	1.80	0.43
1:B:164:ILE:HD13	1:B:322:GLN:HG2	2.01	0.43
1:A:3:GLU:HG3	1:A:274:LYS:NZ	2.35	0.42
1:B:10:VAL:HG22	1:B:40:LYS:HD2	2.01	0.42
1:B:55:ASN:HD22	1:B:58:GLN:HG2	1.84	0.42
1:A:362:VAL:HG12	1:A:389:LEU:HD11	1.98	0.41
1:A:11:ARG:O	1:A:199:ILE:HA	2.20	0.41
1:A:164:ILE:CD1	1:A:379:ILE:CD1	2.97	0.41
1:B:164:ILE:HD11	1:B:379:ILE:CD1	2.49	0.41
1:B:55:ASN:ND2	1:B:58:GLN:HG2	2.36	0.41
1:A:157:MET:HE2	4:A:690:HOH:O	2.21	0.40
1:B:124:LEU:HB2	1:B:140:VAL:HB	2.03	0.40
1:B:55:ASN:HD21	1:B:61:LEU:HD12	1.85	0.40
1:B:314:GLU:HG3	1:B:361:LEU:HB2	2.03	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	390/400 (98%)	374 (96%)	13 (3%)	3 (1%)	19	7
1	B	390/400 (98%)	374 (96%)	12 (3%)	4 (1%)	15	4
All	All	780/800 (98%)	748 (96%)	25 (3%)	7 (1%)	17	5

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	284	ASP
1	A	87	VAL
1	A	350	ILE
1	B	87	VAL
1	A	284	ASP
1	B	350	ILE
1	B	381	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	294/302 (97%)	291 (99%)	3 (1%)	76	68
1	B	294/302 (97%)	287 (98%)	7 (2%)	49	33
All	All	588/604 (97%)	578 (98%)	10 (2%)	60	48

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	92	LEU
1	A	155	TYR
1	B	1	MET
1	B	22	LYS
1	B	92	LEU
1	B	155	TYR
1	B	262	GLU
1	B	287	ILE
1	B	288	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	250	ASN
1	B	55	ASN
1	B	58	GLN
1	B	63	GLN
1	B	250	ASN
1	B	322	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	ACT	B	402	-	1,3,3	0.60	0	0,3,3	0.00	-
2	ACT	B	401	-	1,3,3	0.01	0	0,3,3	0.00	-
2	ACT	A	401	-	1,3,3	0.87	0	0,3,3	0.00	-
2	ACT	A	402	-	1,3,3	3.16	1 (100%)	0,3,3	0.00	-
3	GOL	B	403	-	5,5,5	0.44	0	5,5,5	0.61	0
3	GOL	B	404	-	5,5,5	0.79	0	5,5,5	0.74	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	GOL	B	403	-	-	4/4/4/4	-
3	GOL	B	404	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	402	ACT	CH3-C	3.16	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	GOL	O1-C1-C2-O2
3	B	403	GOL	O1-C1-C2-C3
3	B	403	GOL	C1-C2-C3-O3
3	B	404	GOL	O1-C1-C2-C3
3	B	403	GOL	O2-C2-C3-O3
3	B	404	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	GOL	3	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	392/400 (98%)	0.56	28 (7%) 16 15	15, 25, 55, 119	0
1	B	392/400 (98%)	0.68	41 (10%) 6 6	16, 26, 59, 134	0
All	All	784/800 (98%)	0.62	69 (8%) 10 9	15, 25, 58, 134	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	287	ILE	17.6
1	B	285	PRO	16.6
1	A	287	ILE	15.4
1	A	283	VAL	13.2
1	B	286	ALA	13.1
1	A	286	ALA	12.2
1	B	283	VAL	11.1
1	A	289	GLY	10.7
1	B	207	ARG	10.6
1	A	290	TYR	10.3
1	B	288	MET	10.3
1	A	285	PRO	10.2
1	B	284	ASP	9.4
1	B	290	TYR	9.3
1	A	207	ARG	9.0
1	B	206	GLY	7.8
1	B	289	GLY	7.2
1	B	209	GLY	7.0
1	B	282	GLY	6.9
1	B	208	LYS	6.6
1	A	288	MET	6.1
1	A	284	ASP	5.7
1	A	208	LYS	5.5
1	A	282	GLY	5.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	1	MET	4.5
1	B	84	ILE	3.9
1	B	232	LYS	3.9
1	B	152	PHE	3.7
1	A	230	LYS	3.5
1	B	381	GLY	3.4
1	A	84	ILE	3.4
1	B	51	VAL	3.3
1	A	281	ALA	3.3
1	A	294	TYR	3.2
1	B	81	ALA	3.2
1	A	209	GLY	3.2
1	B	281	ALA	3.1
1	B	210	GLU	3.0
1	B	294	TYR	2.9
1	A	152	PHE	2.8
1	B	234	ALA	2.8
1	B	53	LEU	2.8
1	A	133	ARG	2.7
1	A	56	VAL	2.7
1	A	232	LYS	2.7
1	B	304	GLY	2.6
1	A	83	THR	2.6
1	A	168	TRP	2.5
1	B	230	LYS	2.5
1	B	27	VAL	2.5
1	B	83	THR	2.5
1	A	1	MET	2.4
1	A	52	ILE	2.4
1	B	237	LYS	2.4
1	A	234	ALA	2.4
1	B	52	ILE	2.3
1	B	112	ALA	2.3
1	B	205	LYS	2.3
1	B	34	ILE	2.3
1	A	235	PHE	2.2
1	B	291	GLY	2.2
1	B	71	PHE	2.1
1	B	151	ALA	2.1
1	B	79	ILE	2.1
1	A	239	GLY	2.1
1	B	110	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	95	VAL	2.0
1	B	111	ILE	2.0
1	B	80	PRO	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	B	404	6/6	0.69	0.18	46,54,55,56	0
3	GOL	B	403	6/6	0.85	0.15	42,53,56,56	0
2	ACT	B	402	4/4	0.86	0.13	34,38,48,55	0
2	ACT	A	402	4/4	0.91	0.11	39,47,51,53	0
2	ACT	B	401	4/4	0.95	0.17	19,23,24,27	1
2	ACT	A	401	4/4	0.96	0.18	23,25,27,27	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.