



# Full wwPDB X-ray Structure Validation Report

Mar 26, 2014 – 06:14 PM EDT

PDB ID : 4ONC  
Title : Crystal Structure of Mycobacterium Tuberculosis Decaprenyl Diphosphate Synthase in Complex with BPH-640  
Authors : Feng, X.; Chan, H.C.; Ko, T.P.  
Deposited on : 2014-01-28  
Resolution : 1.83 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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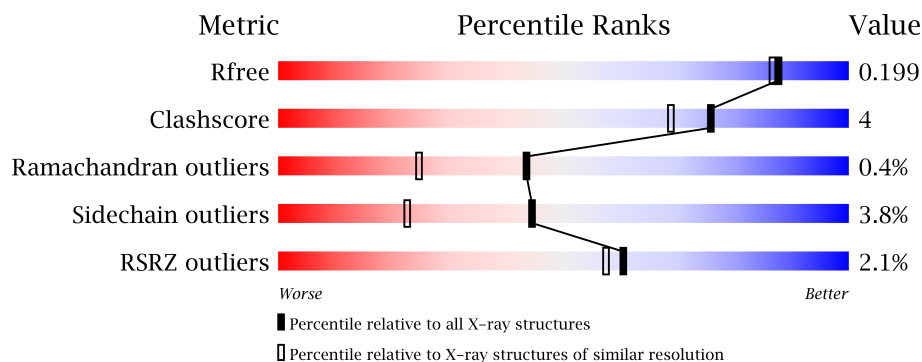
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 1.83 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))
$R_{free}$	66092	1857 (1.86-1.82)
Clashscore	79885	2149 (1.86-1.82)
Ramachandran outliers	78287	2124 (1.86-1.82)
Sidechain outliers	78261	2125 (1.86-1.82)
RSRZ outliers	66119	1857 (1.86-1.82)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	284	
1	B	284	

## 2 Entry composition i

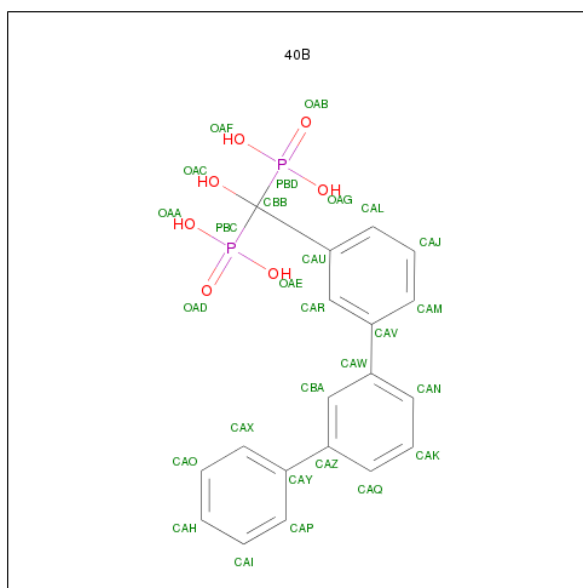
There are 3 unique types of molecules in this entry. The entry contains 4991 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Decaprenyl diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2238	1410	415	404	9			
1	B	282	Total	C	N	O	S	0	0	0
			2272	1432	420	411	9			

- Molecule 2 is [HYDROXY(1,1':3',1''-TERPHENYL-3-YL)METHANEDIYL]BIS(PHOSPHONICACID) (three-letter code: 40B) (formula: C<sub>19</sub>H<sub>18</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			28	19	7	2		
2	B	1	Total	C	O	P	0	0
			16	7	7	2		

- Molecule 3 is water.

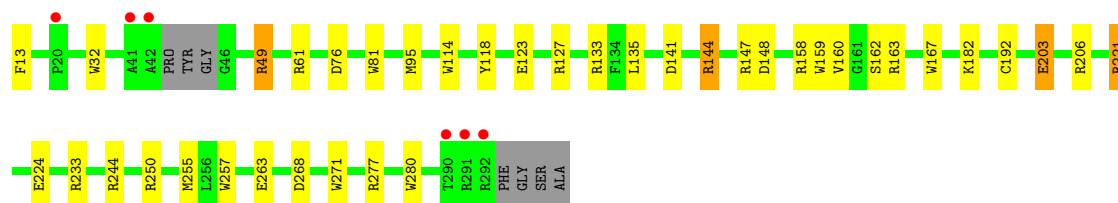
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	219	Total 219	O 219	0	0
3	B	218	Total 218	O 218	0	0

### 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 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.

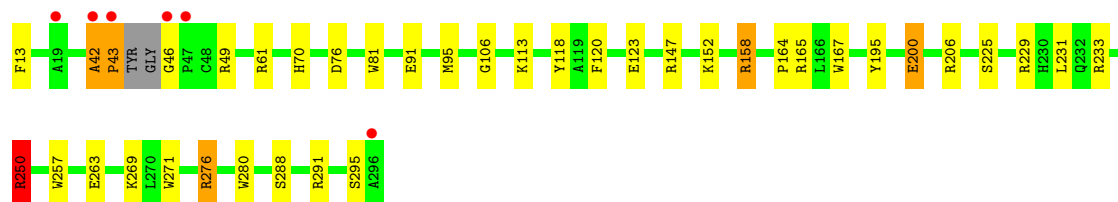
- Molecule 1: Decaprenyl diphosphate synthase

Chain A: 



- Molecule 1: Decaprenyl diphosphate synthase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.81Å 89.17Å 93.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 1.83 49.73 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.73-1.83) 100.0 (49.73-1.83)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.157 , 0.198 0.158 , 0.199	Depositor DCC
$R_{free}$ test set	2945 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.1	EDS
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 58301 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4991	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 40B

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	1.23	11/2296 (0.5%)	1.17	11/3122 (0.4%)
1	B	1.30	9/2332 (0.4%)	1.18	11/3170 (0.3%)
All	All	1.27	20/4628 (0.4%)	1.17	22/6292 (0.3%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	271	TRP	CD2-CE2	7.08	1.49	1.41
1	A	114	TRP	CD2-CE2	6.78	1.49	1.41
1	A	203	GLU	CG-CD	6.43	1.61	1.51
1	B	200	GLU	CD-OE2	-6.26	1.18	1.25
1	A	257	TRP	CD2-CE2	6.12	1.48	1.41
1	B	257	TRP	CD2-CE2	6.10	1.48	1.41
1	B	70	HIS	CG-CD2	6.05	1.46	1.35
1	B	81	TRP	CD2-CE2	5.80	1.48	1.41
1	B	167	TRP	CD2-CE2	5.77	1.48	1.41
1	A	224	GLU	CD-OE2	5.63	1.31	1.25
1	A	159	TRP	CD2-CE2	5.60	1.48	1.41
1	A	280	TRP	CD2-CE2	5.59	1.48	1.41
1	B	276	ARG	CZ-NH2	5.44	1.40	1.33
1	A	49	ARG	CZ-NH1	5.34	1.40	1.33
1	A	123	GLU	CG-CD	5.22	1.59	1.51
1	A	167	TRP	CD2-CE2	5.22	1.47	1.41
1	A	271	TRP	CG-CD1	5.17	1.44	1.36
1	B	280	TRP	CD2-CE2	5.17	1.47	1.41
1	B	120	PHE	CG-CD2	5.09	1.46	1.38
1	A	159	TRP	CG-CD1	5.03	1.43	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	MET	CG-SD-CE	-10.74	83.01	100.20
1	B	233	ARG	NE-CZ-NH1	-8.92	115.84	120.30
1	B	158	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	B	147	ARG	NE-CZ-NH1	-8.30	116.15	120.30
1	A	244	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	B	158	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	B	291	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	42	ALA	C-N-CD	-6.79	105.66	120.60
1	A	163	ARG	CG-CD-NE	-6.74	97.65	111.80
1	A	144	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	B	147	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	A	127	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	224	GLU	OE1-CD-OE2	6.05	130.56	123.30
1	B	42	ALA	C-N-CA	5.84	146.54	122.00
1	B	42	ALA	N-CA-C	5.77	126.58	111.00
1	A	163	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	A	32	TRP	CA-CB-CG	-5.54	103.18	113.70
1	B	250	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	A	206	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	268	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	277	ARG	NE-CZ-NH1	-5.05	117.77	120.30
1	B	76	ASP	CB-CG-OD1	-5.04	113.77	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2238	0	2203	15	0
1	B	2272	0	2232	21	0
2	A	28	0	0	0	0
2	B	16	0	0	1	0
3	A	219	0	0	3	0
3	B	218	0	0	12	0
All	All	4991	0	4435	35	0



Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (35) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:288:SER:HB2	3:B:677:HOH:O	1.38	1.18
1:A:13:PHE:N	3:A:753:HOH:O	1.78	1.11
1:B:288:SER:CB	3:B:677:HOH:O	1.92	1.04
1:B:95:MET:HE2	3:B:795:HOH:O	1.69	0.92
1:A:263:GLU:OE2	1:B:250:ARG:NH2	2.08	0.86
2:B:500:40B:CAJ	3:B:810:HOH:O	2.28	0.81
1:A:221:ARG:CG	1:A:221:ARG:HH11	1.94	0.80
1:B:13:PHE:N	3:B:742:HOH:O	2.17	0.78
1:A:221:ARG:HG2	1:A:221:ARG:NH1	2.00	0.77
1:A:221:ARG:HG2	1:A:221:ARG:HH11	1.51	0.76
1:B:95:MET:CE	3:B:795:HOH:O	2.30	0.71
1:A:148:ASP:OD1	3:A:791:HOH:O	2.12	0.66
1:B:13:PHE:N	3:B:727:HOH:O	2.33	0.60
1:B:152:LYS:NZ	3:B:798:HOH:O	2.36	0.58
1:B:250:ARG:NH1	3:B:688:HOH:O	2.41	0.53
1:B:288:SER:HB3	3:B:677:HOH:O	1.79	0.53
1:A:203:GLU:HG2	3:A:782:HOH:O	2.08	0.52
1:B:91:GLU:O	1:B:95:MET:HG2	2.10	0.52
1:B:95:MET:HE3	3:B:730:HOH:O	2.09	0.51
1:B:295:SER:HB3	3:B:617:HOH:O	2.09	0.51
1:A:160:VAL:HG22	1:A:233:ARG:HG3	1.93	0.51
1:B:106:GLY:HA3	1:B:276:ARG:HB2	1.92	0.51
1:A:141:ASP:OD1	1:A:144:ARG:NH2	2.45	0.49
1:B:225:SER:HB3	1:B:229:ARG:NH1	2.26	0.49
1:A:81:TRP:CH2	1:A:95:MET:HG3	2.48	0.49
1:B:195:TYR:CD1	1:B:195:TYR:C	2.86	0.48
1:A:221:ARG:HG3	1:A:221:ARG:HH11	1.79	0.46
1:B:113:LYS:HA	1:B:113:LYS:HD2	1.75	0.46
1:A:160:VAL:O	1:A:192:CYS:HA	2.18	0.43
1:B:200:GLU:HG2	1:B:231:LEU:HD22	2.01	0.43
1:A:250:ARG:HD3	1:B:263:GLU:OE2	2.19	0.43
1:A:135:LEU:HD23	1:A:135:LEU:HA	1.80	0.42
1:A:61:ARG:HD3	1:A:61:ARG:HA	1.63	0.42
1:B:61:ARG:HA	1:B:61:ARG:HD3	1.66	0.42
1:B:43:PRO:O	1:B:46:GLY:N	2.53	0.41

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	273/284 (96%)	268 (98%)	5 (2%)	0	100	100
1	B	278/284 (98%)	272 (98%)	4 (1%)	2 (1%)	30	12
All	All	551/568 (97%)	540 (98%)	9 (2%)	2 (0%)	43	25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	42	ALA
1	B	165	ARG

### 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	235/239 (98%)	226 (96%)	9 (4%)	44	22
1	B	238/239 (100%)	229 (96%)	9 (4%)	44	22
All	All	473/478 (99%)	455 (96%)	18 (4%)	44	22

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	76	ASP
1	A	118	TYR
1	A	133	ARG
1	A	147	ARG
1	A	158	ARG
1	A	162	SER

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Mol	Chain	Res	Type
1	A	182	LYS
1	A	221	ARG
1	B	43	PRO
1	B	49	ARG
1	B	118	TYR
1	B	123	GLU
1	B	158	ARG
1	B	164	PRO
1	B	206	ARG
1	B	250	ARG
1	B	269	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	249	GLN
1	B	69	ASN
1	B	249	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	40B	A	500	-	30,30,30	2.79	11 (36%)	46,46,46	2.04	13 (28%)
2	40B	B	500	-	16,16,30	3.66	9 (56%)	25,26,46	2.62	9 (36%)

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	40B	A	500	-	-	0/32/32/32	0/3/3/3
2	40B	B	500	-	-	0/24/24/32	0/1/1/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	40B	PBC-OAD	9.54	1.66	1.50
2	B	500	40B	PBD-OAB	6.79	1.61	1.50
2	B	500	40B	PBC-OAE	6.51	1.67	1.54
2	B	500	40B	PBD-OAG	6.19	1.66	1.54
2	A	500	40B	PBD-CBB	4.90	1.93	1.85
2	B	500	40B	PBC-CBB	-4.90	1.76	1.85
2	A	500	40B	PBD-OAG	4.29	1.63	1.54
2	B	500	40B	CBB-CAU	-3.89	1.45	1.53
2	A	500	40B	CBB-CAU	-3.65	1.45	1.53
2	A	500	40B	PBD-OAB	3.56	1.56	1.50
2	B	500	40B	PBD-CBB	3.54	1.91	1.85
2	B	500	40B	PBC-OAA	3.52	1.61	1.54
2	B	500	40B	PBC-OAD	3.42	1.56	1.50
2	A	500	40B	PBC-OAE	2.96	1.60	1.54
2	A	500	40B	PBC-OAA	-2.89	1.49	1.54
2	A	500	40B	CAR-CAU	2.76	1.44	1.39
2	A	500	40B	PBC-CBB	2.28	1.89	1.85
2	A	500	40B	CAY-CAZ	-2.27	1.42	1.49
2	A	500	40B	CAM-CAV	2.18	1.44	1.39
2	B	500	40B	PBD-OAF	-2.09	1.50	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	40B	OAF-PBD-CBB	7.06	116.27	104.73
2	B	500	40B	PBD-CBB-PBC	-6.88	106.27	114.34
2	B	500	40B	OAG-PBD-CBB	-5.70	95.40	104.73
2	B	500	40B	OAF-PBD-CBB	5.49	113.72	104.73
2	A	500	40B	OAE-PBC-CBB	4.49	112.07	104.73
2	A	500	40B	OAA-PBC-CBB	4.49	112.07	104.73
2	A	500	40B	OAB-PBD-CBB	-3.78	101.38	110.95
2	B	500	40B	OAG-PBD-OAF	3.62	118.24	107.93
2	A	500	40B	OAD-PBC-CBB	-3.61	101.82	110.95
2	B	500	40B	OAE-PBC-CBB	-2.93	99.93	104.73
2	B	500	40B	OAF-PBD-OAB	-2.74	107.02	113.14
2	A	500	40B	OAG-PBD-OAB	-2.66	107.19	113.14
2	B	500	40B	PBD-CBB-CAU	2.63	115.05	110.22
2	A	500	40B	CAN-CAW-CAV	-2.59	116.84	121.41
2	A	500	40B	CBA-CAW-CAV	2.57	125.41	120.89
2	B	500	40B	OAA-PBC-OAD	2.47	118.66	113.14
2	A	500	40B	CAR-CAU-CBB	-2.44	117.90	120.77
2	A	500	40B	CAJ-CAL-CAU	-2.31	118.09	120.75
2	A	500	40B	CAL-CAU-CAR	2.30	122.01	117.59
2	A	500	40B	OAG-PBD-OAF	2.23	114.29	107.93
2	A	500	40B	PBD-CBB-PBC	-2.21	111.75	114.34
2	B	500	40B	CAL-CAU-CBB	2.01	123.13	120.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	277/284 (97%)	-0.17	6 (2%) 59 56	15, 25, 46, 92	0
1	B	282/284 (99%)	-0.38	6 (2%) 60 57	14, 23, 42, 71	0
All	All	559/568 (98%)	-0.28	12 (2%) 60 57	14, 24, 45, 92	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	THR	6.1
1	A	292	ARG	4.6
1	A	291	ARG	4.2
1	B	43	PRO	3.4
1	B	42	ALA	3.2
1	A	42	ALA	2.8
1	B	46	GLY	2.7
1	B	47	PRO	2.3
1	B	296	ALA	2.3
1	A	41	ALA	2.2
1	A	20	PRO	2.2
1	B	19	ALA	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	40B	A	500	28/28	0.12	1.92	22,32,62,64	0
2	40B	B	500	16/28	0.15	1.72	31,55,67,68	0

## 6.5 Other polymers

There are no such residues in this entry.