



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 11:56 am BST

PDB ID : 1W27  
Title : Phenylalanine ammonia-lyase (PAL) from Petroselinum crispum  
Authors : Ritter, H.; Schulz, G.E.  
Deposited on : 2004-06-29  
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

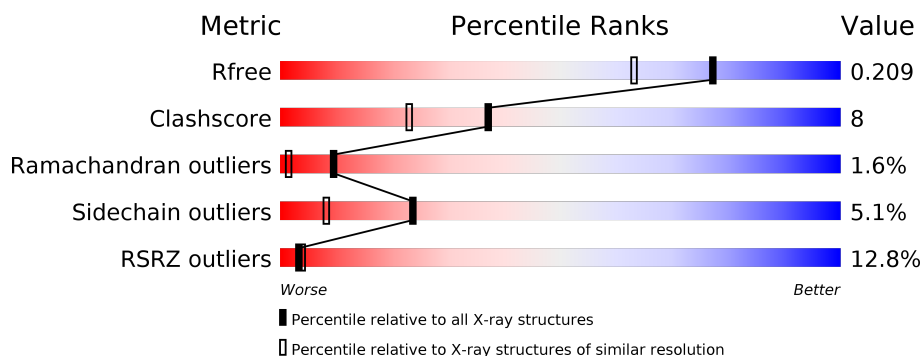
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	714	<div> <div>11%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>
1	B	714	<div> <div>13%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• •</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11663 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.

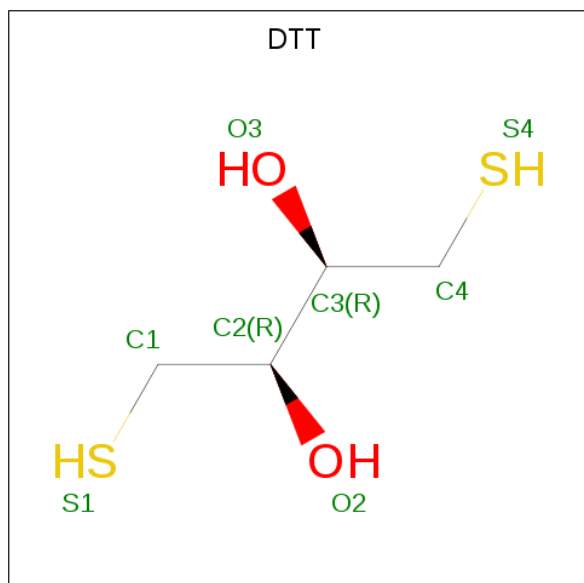
- Molecule 1 is a protein called PHENYLALANINE AMMONIA-LYASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	690	Total	C	N	O	S	0	0	0
			5288	3335	912	1014	27			
1	B	690	Total	C	N	O	S	0	0	0
			5288	3335	912	1014	27			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	MDO	ALA	modified residue	UNP P24481
A	203	MDO	SER	modified residue	UNP P24481
A	203	MDO	GLY	modified residue	UNP P24481
B	203	MDO	ALA	modified residue	UNP P24481
B	203	MDO	SER	modified residue	UNP P24481
B	203	MDO	GLY	modified residue	UNP P24481

- Molecule 2 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			8	4	2	2		
2	B	1	Total	C	O	S	0	0
			8	4	2	2		

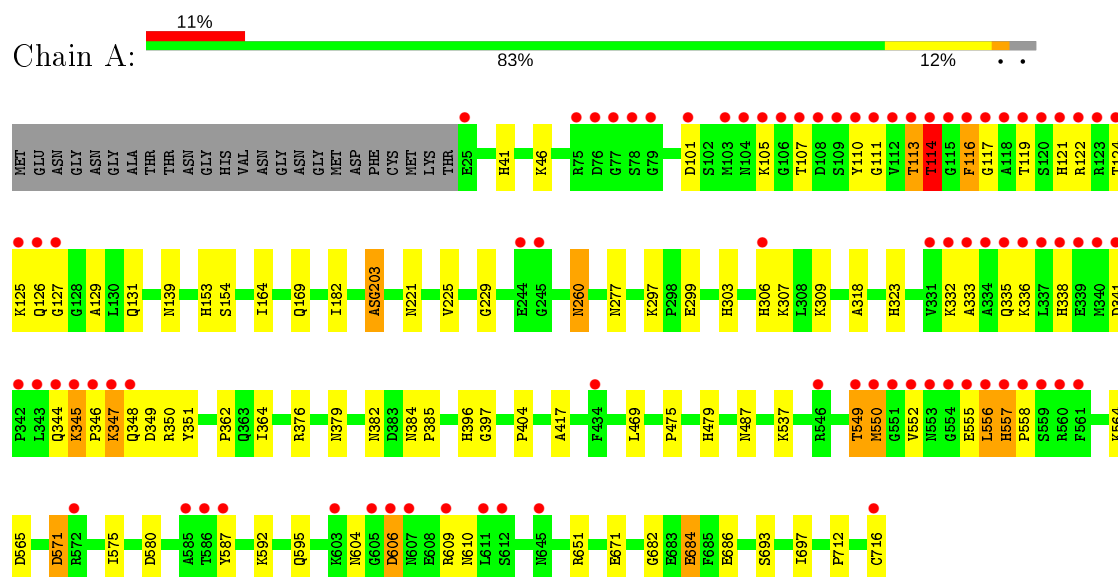
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	534	Total	O	0	0
			534	534		
3	B	537	Total	O	0	0
			537	537		

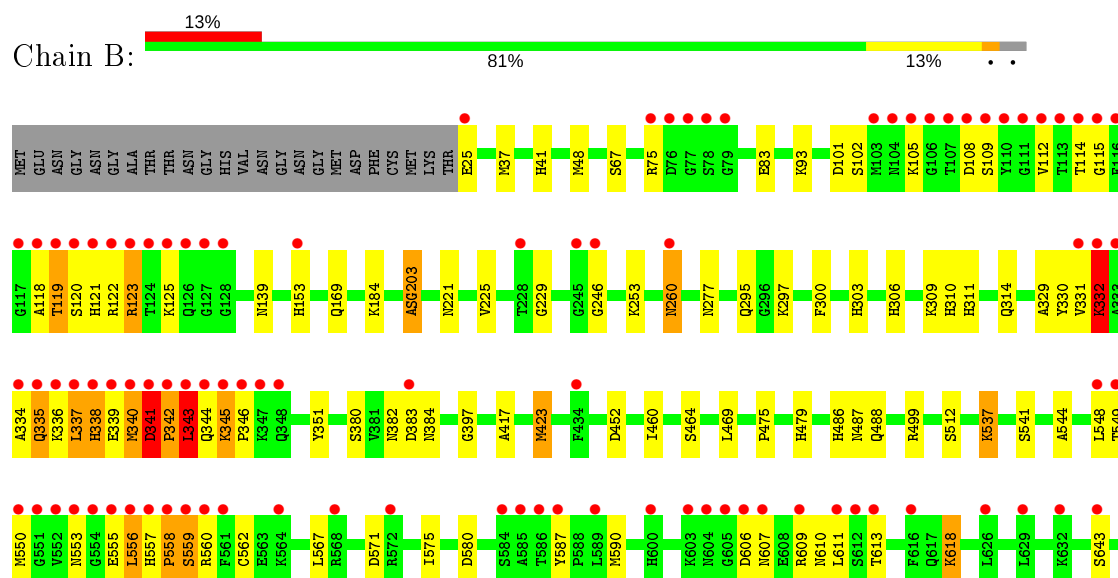
### 3 Residue-property plots [i](#)

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: PHENYLALANINE AMMONIA-LYASE 1



#### • Molecule 1: PHENYLALANINE AMMONIA-LYASE 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.96Å 160.81Å 141.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 19.98 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-1.70) 98.4 (19.98-1.70)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.82 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.166 , 0.199 0.180 , 0.209	Depositor DCC
$R_{free}$ test set	7349 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11663	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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: MDO, DTT

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	0/5369	0.74	5/7264 (0.1%)
1	B	0.57	1/5369 (0.0%)	0.73	7/7264 (0.1%)
All	All	0.56	1/10738 (0.0%)	0.74	12/14528 (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	A	0	2
1	B	0	4
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	423	MET	SD-CE	-10.63	1.18	1.77

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	ASP	CB-CG-OD2	6.38	124.04	118.30
1	B	580	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	101	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	341	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	101	ASP	CB-CG-OD2	5.56	123.31	118.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	203	MDO	Mainchain,Peptide
1	B	203	MDO	Mainchain,Peptide
1	B	246	GLY	Peptide
1	B	340	MET	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	5288	0	5317	79	0
1	B	5288	0	5317	99	2
2	A	8	0	9	1	0
2	B	8	0	9	1	0
3	A	534	0	0	18	1
3	B	537	0	0	28	1
All	All	11663	0	10652	166	3

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 8.

The worst 5 of 166 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:423:MET:SD	1:B:423:MET:CE	1.18	1.27
1:B:423:MET:SD	1:B:423:MET:HE2	1.76	1.14
1:B:423:MET:SD	1:B:423:MET:HE1	1.76	1.13
1:B:423:MET:HE3	1:B:423:MET:SD	1.76	1.10
1:A:306:HIS:HD2	1:A:318:ALA:CB	1.66	1.08

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:HIS:ND1	1:B:486:HIS:ND1[3_555]	2.05	0.15
1:B:486:HIS:ND1	1:B:486:HIS:CE1[3_555]	2.11	0.09
3:A:2510:HOH:O	3:B:2131:HOH:O[3_555]	2.18	0.02

## 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	687/714 (96%)	648 (94%)	28 (4%)	11 (2%)	9	1
1	B	687/714 (96%)	644 (94%)	32 (5%)	11 (2%)	9	1
All	All	1374/1428 (96%)	1292 (94%)	60 (4%)	22 (2%)	9	1

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	THR
1	B	338	HIS
1	B	341	ASP
1	B	342	PRO
1	B	556	LEU

### 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	573/591 (97%)	548 (96%)	25 (4%)	28	11
1	B	573/591 (97%)	540 (94%)	33 (6%)	20	6
All	All	1146/1182 (97%)	1088 (95%)	58 (5%)	24	8

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	93	LYS

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Mol	Chain	Res	Type
1	B	120	SER
1	B	610	ASN
1	B	102	SER
1	B	109	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	595	GLN
1	B	145	ASN
1	B	591	GLN
1	B	41	HIS
1	B	153	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	MDO	A	203	1,2	12,13,14	2.12	3 (25%)	15,18,20	3.84	6 (40%)
1	MDO	B	203	1,2	12,13,14	2.39	5 (41%)	15,18,20	3.67	7 (46%)

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
1	MDO	A	203	1,2	-	1/4/23/24	0/1/1/1
1	MDO	B	203	1,2	-	2/4/23/24	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	MDO	O2-C2	5.11	1.33	1.23
1	B	203	MDO	O2-C2	5.05	1.33	1.23
1	B	203	MDO	C2-N3	-3.92	1.30	1.39
1	A	203	MDO	C2-N3	-3.61	1.31	1.39
1	B	203	MDO	C1-N3	-2.71	1.32	1.37

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	MDO	CA2-C2-N3	11.77	108.93	103.37
1	A	203	MDO	CA2-C2-N3	11.49	108.80	103.37
1	A	203	MDO	O2-C2-CA2	-5.86	127.67	130.96
1	A	203	MDO	C2-CA2-N2	-4.80	105.57	108.93
1	B	203	MDO	C2-CA2-N2	-4.00	106.13	108.93

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	203	MDO	N2-C1-CA-CB
1	B	203	MDO	N2-C1-CA-CB
1	B	203	MDO	N3-C1-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	203	MDO	1	0
1	B	203	MDO	1	0

## 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	DTT	B	1717	1	7,7,7	0.69	0	4,8,8	1.26	0
2	DTT	A	1717	1	7,7,7	0.83	0	4,8,8	0.53	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
2	DTT	B	1717	1	-	0/8/8/8	-
2	DTT	A	1717	1	-	1/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1717	DTT	S1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1717	DTT	1	0
2	A	1717	DTT	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	689/714 (96%)	0.88	81 (11%) 4 5	11, 20, 56, 63	0
1	B	689/714 (96%)	1.07	96 (13%) 2 3	11, 20, 57, 62	0
All	All	1378/1428 (96%)	0.97	177 (12%) 3 4	11, 20, 57, 63	0

The worst 5 of 177 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	343	LEU	20.7
1	A	112	VAL	18.6
1	B	118	ALA	18.3
1	B	337	LEU	17.8
1	A	343	LEU	17.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	MDO	A	203	13/14	0.92	0.09	14,15,20,27	0
1	MDO	B	203	13/14	0.94	0.09	13,15,19,29	0

### 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( $\text{\AA}^2$ )	Q<0.9
2	DTT	B	1717	8/8	0.88	0.15	34,40,42,43	0
2	DTT	A	1717	8/8	0.93	0.14	30,35,37,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.