



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:22 PM GMT

PDB ID : 5CYI  
Title : CDK2/Cyclin A covalent complex with 6-(cyclohexylmethoxy)-N-(4-(vinylsulfonyl)phenyl)-9H-purin-2-amine (NU6300)  
Authors : Anscombe, E.; Meschini, E.; Vidal, R.M.; Martin, M.P.; Staunton, D.; Geitmann, M.; Danielson, U.H.; Stanley, W.A.; Wang, L.Z.; Reuillon, T.; Golding, B.T.; Cano, C.; Newell, D.R.; Noble, M.E.M.; Wedge, S.R.; Endicott, J.A.; Griffin, R.J.  
Deposited on : 2015-07-30  
Resolution : 2.00 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20026982

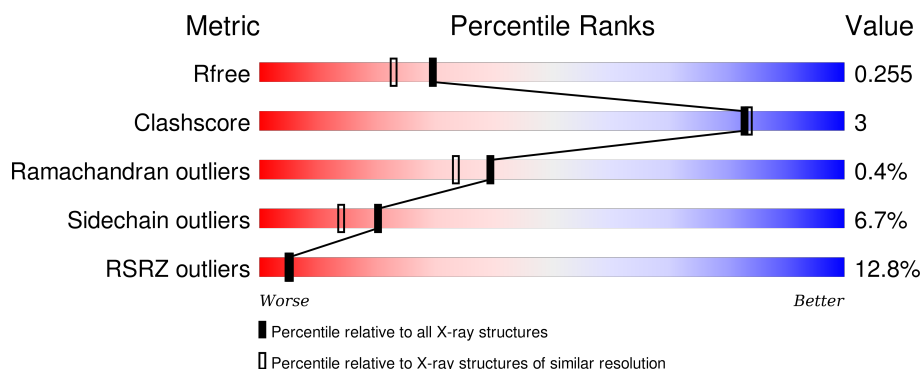
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	303	<div> <div>4%</div> <div>82%</div> <div>13%</div> <div>• •</div> </div>
1	C	303	<div> <div>21%</div> <div>86%</div> <div>12%</div> <div>•</div> </div>
2	B	260	<div> <div>2%</div> <div>91%</div> <div>6%</div> <div>• •</div> </div>
2	D	260	<div> <div>23%</div> <div>91%</div> <div>7%</div> <div>• •</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9513 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 Cyclin-dependent kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	P	S	0	1	0
			2414	1567	410	428	1	8			
1	C	297	Total	C	N	O	P	S	0	1	0
			2397	1555	405	428	1	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P24941
A	-3	PRO	-	expression tag	UNP P24941
A	-2	LEU	-	expression tag	UNP P24941
A	-1	GLY	-	expression tag	UNP P24941
A	0	SER	-	expression tag	UNP P24941
C	-4	GLY	-	expression tag	UNP P24941
C	-3	PRO	-	expression tag	UNP P24941
C	-2	LEU	-	expression tag	UNP P24941
C	-1	GLY	-	expression tag	UNP P24941
C	0	SER	-	expression tag	UNP P24941

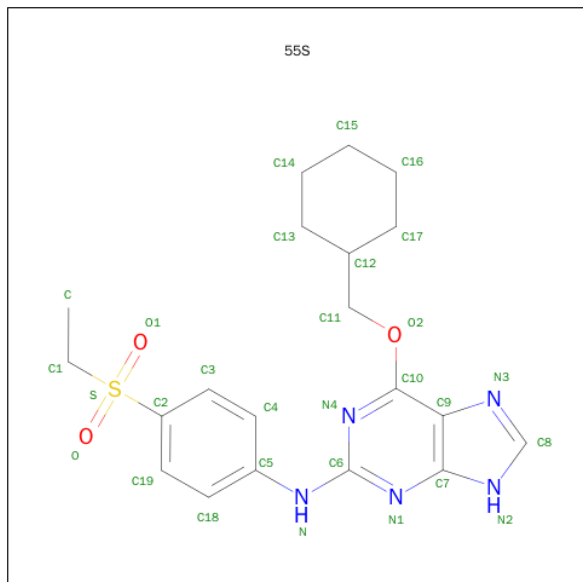
- Molecule 2 is a protein called Cyclin-A2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S		0	0	0
			2083	1350	339	383	11				
2	D	256	Total	C	N	O	S		0	0	0
			2069	1340	337	381	11				

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	173	MET	-	initiating methionine	UNP P20248
D	173	MET	-	initiating methionine	UNP P20248

- Molecule 3 is 6-(cyclohexylmethoxy)-N-[4-(ethylsulfonyl)phenyl]-9H-purin-2-amine (three-letter code: 55S) (formula: C<sub>20</sub>H<sub>25</sub>N<sub>5</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			29	20	5	3	1		
3	C	1	Total	C	N	O	S	0	0
			29	20	5	3	1		

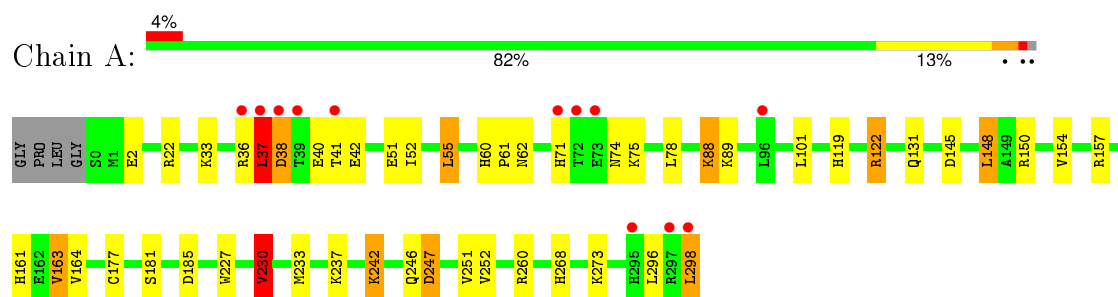
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	224	Total	O	0	0
			224	224		
4	B	166	Total	O	0	0
			166	166		
4	C	64	Total	O	0	0
			64	64		
4	D	38	Total	O	0	0
			38	38		

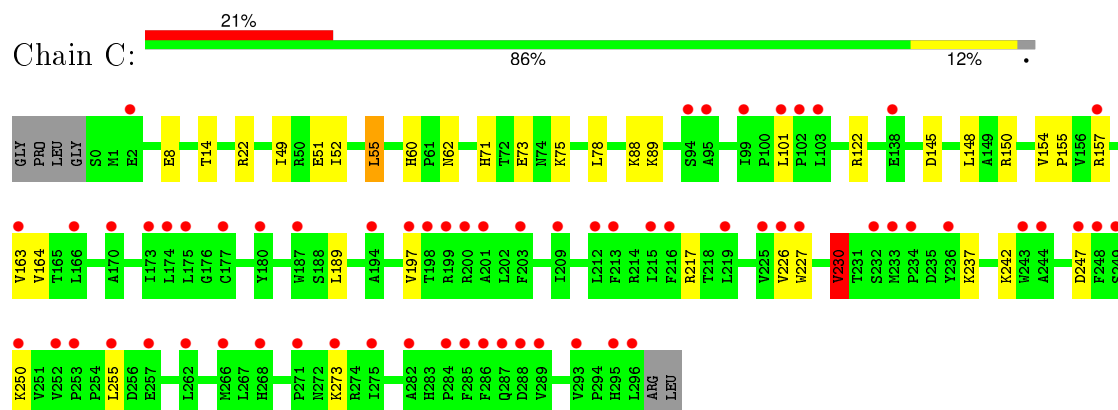
### 3 Residue-property plots [i](#)

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

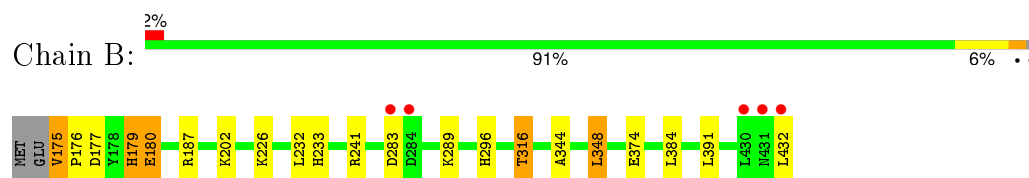
#### • Molecule 1: Cyclin-dependent kinase 2



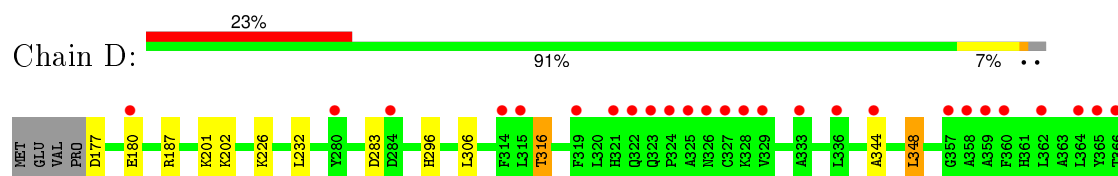
#### • Molecule 1: Cyclin-dependent kinase 2

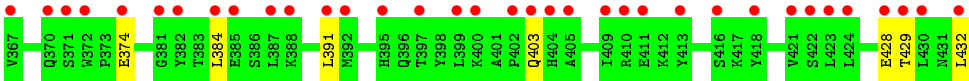


#### • Molecule 2: Cyclin-A2



#### • Molecule 2: Cyclin-A2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.29Å 135.29Å 148.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.34 – 2.00 74.34 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (74.34-2.00) 99.9 (74.34-2.00)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, $R_{free}$	0.227 , 0.255 0.227 , 0.255	Depositor DCC
$R_{free}$ test set	4914 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 101635 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9513	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: TPO, 55S

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	0.74	0/2464	0.97	6/3343 (0.2%)
1	C	0.68	0/2447	0.90	2/3320 (0.1%)
2	B	0.63	1/2133 (0.0%)	0.86	4/2897 (0.1%)
2	D	0.55	0/2118	0.78	2/2875 (0.1%)
All	All	0.66	1/9162 (0.0%)	0.88	14/12435 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	180	GLU	CG-CD	5.00	1.59	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	177	ASP	CB-CG-OD1	11.28	128.45	118.30
1	A	38	ASP	CB-CG-OD1	9.00	126.40	118.30
1	A	148	LEU	CB-CG-CD2	7.97	124.55	111.00
1	A	37	LEU	CB-CG-CD2	7.96	124.53	111.00
1	C	230	VAL	CB-CA-C	-6.74	98.60	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	40	GLU	Peptide
1	A	41	THR	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	2414	0	2459	34	0
1	C	2397	0	2432	15	1
2	B	2083	0	2107	12	0
2	D	2069	0	2091	7	1
3	A	29	0	23	0	0
3	C	29	0	24	0	0
4	A	224	0	0	10	0
4	B	166	0	0	4	0
4	C	64	0	0	0	0
4	D	38	0	0	0	0
All	All	9513	0	9136	56	1

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 3.

The worst 5 of 56 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:148:LEU:HD22	4:A:497:HOH:O	1.76	0.83
1:A:71:HIS:HD2	2:B:296:HIS:NE2	1.80	0.80
1:A:230:VAL:HA	1:A:233:MET:CE	2.13	0.79
1:A:154:VAL:O	2:B:316:THR:CG2	2.40	0.69
1:A:71:HIS:CD2	2:B:296:HIS:NE2	2.59	0.69

All (1) 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:C:8:GLU:OE1	2:D:403:GLN:OE1[3_655]	2.18	0.02

## 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	297/303 (98%)	288 (97%)	7 (2%)	2 (1%)	26	19
1	C	295/303 (97%)	288 (98%)	5 (2%)	2 (1%)	26	19
2	B	256/260 (98%)	255 (100%)	1 (0%)	0	100	100
2	D	254/260 (98%)	253 (100%)	1 (0%)	0	100	100
All	All	1102/1126 (98%)	1084 (98%)	14 (1%)	4 (0%)	39	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	VAL
1	C	164	VAL
1	A	145	ASP
1	C	145	ASP

### 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	264/265 (100%)	242 (92%)	22 (8%)	14	8
1	C	262/265 (99%)	243 (93%)	19 (7%)	17	11
2	B	232/234 (99%)	219 (94%)	13 (6%)	26	20
2	D	230/234 (98%)	218 (95%)	12 (5%)	29	23
All	All	988/998 (99%)	922 (93%)	66 (7%)	20	14

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	316	THR
1	C	22	ARG
2	D	316	THR
2	B	348	LEU
2	B	391	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	183	HIS
2	B	233	HIS
1	C	71	HIS
1	A	272	ASN
2	B	179	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	TPO	A	160	1	7,10,11	1.09	0	10,14,16	1.49	3 (30%)
1	TPO	C	160	1	7,10,11	0.73	0	10,14,16	1.47	2 (20%)

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	TPO	A	160	1	-	0/8/11/13	0/0/0/0
1	TPO	C	160	1	-	0/8/11/13	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	160	TPO	O-C-CA	-2.31	119.39	125.69
1	C	160	TPO	O-C-CA	-2.18	119.72	125.69
1	A	160	TPO	OG1-P-O1P	-2.09	102.50	107.48
1	A	160	TPO	O3P-P-O1P	2.72	119.51	110.63
1	C	160	TPO	O3P-P-O1P	3.30	121.39	110.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
3	55S	A	301	1	28,32,32	1.26	2 (7%)	37,45,45	1.05	4 (10%)
3	55S	C	301	1	28,32,32	0.99	2 (7%)	37,45,45	0.97	4 (10%)

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	55S	A	301	1	-	0/18/26/26	0/4/4/4
3	55S	C	301	1	-	0/18/26/26	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	55S	C5-N	2.07	1.45	1.40
3	C	301	55S	C5-N	2.24	1.45	1.40
3	C	301	55S	O2-C10	3.62	1.37	1.35
3	A	301	55S	O2-C10	5.65	1.38	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	55S	C9-C10-N4	-3.02	120.04	124.09
3	C	301	55S	C9-C7-N2	-2.67	106.39	111.12
3	A	301	55S	C9-C7-N2	-2.64	106.44	111.12
3	C	301	55S	C9-C10-N4	-2.57	120.64	124.09
3	C	301	55S	C6-N4-C10	2.32	118.50	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	298/303 (98%)	0.51	12 (4%) 42 44	20, 32, 76, 119	0
1	C	296/303 (97%)	1.07	64 (21%) 1 1	34, 62, 96, 118	0
2	B	258/260 (99%)	0.09	5 (1%) 70 70	22, 34, 63, 118	0
2	D	256/260 (98%)	1.23	61 (23%) 1 1	31, 69, 118, 139	0
All	All	1108/1126 (98%)	0.73	142 (12%) 5 5	20, 46, 100, 139	0

The worst 5 of 142 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	372	TRP	7.7
2	D	327	CYS	7.7
1	C	296	LEU	7.3
2	D	399	LEU	6.5
2	D	324	PRO	6.4

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

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
1	TPO	C	160	11/12	0.92	0.13	-	45,59,67,70	0
1	TPO	A	160	11/12	0.99	0.12	-	22,27,29,29	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. 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
3	55S	C	301	29/29	0.95	0.13	-0.49	38,48,64,72	0
3	55S	A	301	29/29	0.96	0.12	-0.72	35,40,63,67	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.