



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:44 AM GMT

PDB ID : 3PPZ  
Title : Crystal structure of CTR1 kinase domain in complex with staurosporine  
Authors : Mayerhofer, H.; Panneerselvam, S.; Mueller-Dieckmann, J.  
Deposited on : 2010-11-25  
Resolution : 2.99 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.

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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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

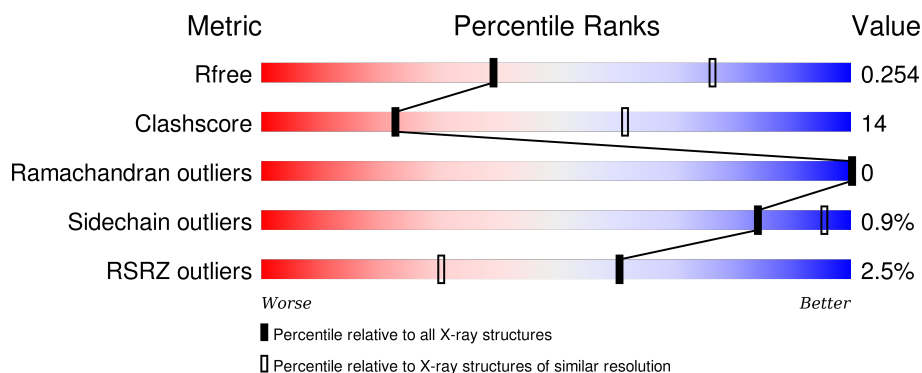
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	309	<div> <div>2%</div> <div>59%</div> <div>27%</div> <div>14%</div> </div>
1	B	309	<div> <div>2%</div> <div>65%</div> <div>20%</div> <div>•</div> <div>14%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4319 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 Serine/threonine-protein kinase CTR1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	P	S	0	0	0
			2132	1350	379	388	3	12			
1	B	267	Total	C	N	O	P	S	0	0	0
			2152	1362	383	392	3	12			

There are 54 discrepancies between the modelled and reference sequences:

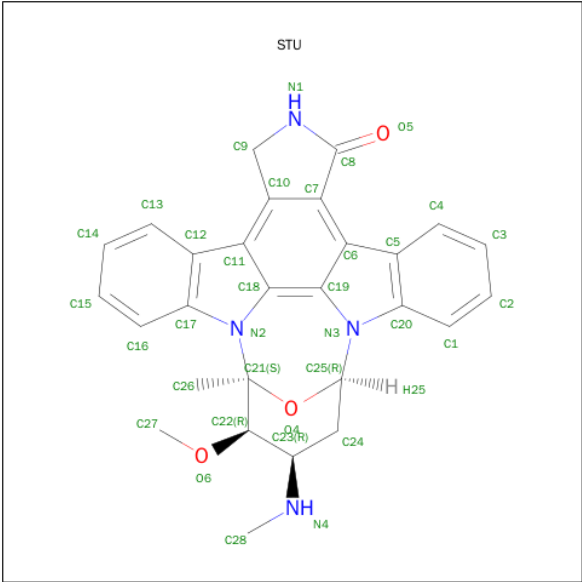
Chain	Residue	Modelled	Actual	Comment	Reference
A	513	MET	-	EXPRESSION TAG	UNP Q05609
A	514	LYS	-	EXPRESSION TAG	UNP Q05609
A	515	HIS	-	EXPRESSION TAG	UNP Q05609
A	516	HIS	-	EXPRESSION TAG	UNP Q05609
A	517	HIS	-	EXPRESSION TAG	UNP Q05609
A	518	HIS	-	EXPRESSION TAG	UNP Q05609
A	519	HIS	-	EXPRESSION TAG	UNP Q05609
A	520	HIS	-	EXPRESSION TAG	UNP Q05609
A	521	PRO	-	EXPRESSION TAG	UNP Q05609
A	522	MET	-	EXPRESSION TAG	UNP Q05609
A	523	SER	-	EXPRESSION TAG	UNP Q05609
A	524	ASP	-	EXPRESSION TAG	UNP Q05609
A	525	TYR	-	EXPRESSION TAG	UNP Q05609
A	526	ASP	-	EXPRESSION TAG	UNP Q05609
A	527	ILE	-	EXPRESSION TAG	UNP Q05609
A	528	PRO	-	EXPRESSION TAG	UNP Q05609
A	529	THR	-	EXPRESSION TAG	UNP Q05609
A	530	THR	-	EXPRESSION TAG	UNP Q05609
A	531	GLU	-	EXPRESSION TAG	UNP Q05609
A	532	ASN	-	EXPRESSION TAG	UNP Q05609
A	533	LEU	-	EXPRESSION TAG	UNP Q05609
A	534	TYR	-	EXPRESSION TAG	UNP Q05609
A	535	PHE	-	EXPRESSION TAG	UNP Q05609
A	536	GLN	-	EXPRESSION TAG	UNP Q05609
A	537	GLY	-	EXPRESSION TAG	UNP Q05609

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Chain	Residue	Modelled	Actual	Comment	Reference
A	538	ALA	-	EXPRESSION TAG	UNP Q05609
A	539	MET	-	EXPRESSION TAG	UNP Q05609
B	513	MET	-	EXPRESSION TAG	UNP Q05609
B	514	LYS	-	EXPRESSION TAG	UNP Q05609
B	515	HIS	-	EXPRESSION TAG	UNP Q05609
B	516	HIS	-	EXPRESSION TAG	UNP Q05609
B	517	HIS	-	EXPRESSION TAG	UNP Q05609
B	518	HIS	-	EXPRESSION TAG	UNP Q05609
B	519	HIS	-	EXPRESSION TAG	UNP Q05609
B	520	HIS	-	EXPRESSION TAG	UNP Q05609
B	521	PRO	-	EXPRESSION TAG	UNP Q05609
B	522	MET	-	EXPRESSION TAG	UNP Q05609
B	523	SER	-	EXPRESSION TAG	UNP Q05609
B	524	ASP	-	EXPRESSION TAG	UNP Q05609
B	525	TYR	-	EXPRESSION TAG	UNP Q05609
B	526	ASP	-	EXPRESSION TAG	UNP Q05609
B	527	ILE	-	EXPRESSION TAG	UNP Q05609
B	528	PRO	-	EXPRESSION TAG	UNP Q05609
B	529	THR	-	EXPRESSION TAG	UNP Q05609
B	530	THR	-	EXPRESSION TAG	UNP Q05609
B	531	GLU	-	EXPRESSION TAG	UNP Q05609
B	532	ASN	-	EXPRESSION TAG	UNP Q05609
B	533	LEU	-	EXPRESSION TAG	UNP Q05609
B	534	TYR	-	EXPRESSION TAG	UNP Q05609
B	535	PHE	-	EXPRESSION TAG	UNP Q05609
B	536	GLN	-	EXPRESSION TAG	UNP Q05609
B	537	GLY	-	EXPRESSION TAG	UNP Q05609
B	538	ALA	-	EXPRESSION TAG	UNP Q05609
B	539	MET	-	EXPRESSION TAG	UNP Q05609

- Molecule 2 is STAUROSPORINE (three-letter code: STU) (formula: C<sub>28</sub>H<sub>26</sub>N<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	28	4	3		

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.

Chain A:

2%

59%

27%

14%

PRO  
PRO  
PRO  
ASN  
ARG  
SER  
ASP  
LEU

P680  
M681  
L682  
L683  
V684  
D685

T689  
V690  
K691  
V692  
C693  
D694

R699  
L700  
K701

L706  
S707  
S708  
K709  
S710  
A711

T714

M718

E721  
V722

E726  
P727  
S728  
N729  
E730

L744

N753  
L754  
P755  
P756

N790  
E791  
P792

F798

M802

R806  
P807

K810

SER  
ALA  
VAL

R595  
E596  
V597

M600  
K601  
R602  
L603  
R604  
H605  
P606  
M607  
I608  
V609  
L610  
F611

P618  
P619  
N620  
L621  
S622

T625

L628  
S629  
R630

L633  
Y634  
R635  
L636  
L637  
H638

K639  
S640  
G641

M654  
A655  
V656  
D657  
V658  
A659  
K660  
G661  
M662

L665

R668  
M669  
P670

R675

K678  
S679

MET  
LYS  
HIS  
HIS  
HIS  
HIS  
PRO  
MET  
SER  
ASP  
TYR  
ASP  
ILE  
PRO  
THR  
THR  
GLU  
ASN  
LEU  
TYR  
PHE  
GLN  
GLY  
ALA  
MET

D540

M544  
D545  
T546  
P547  
V548

K554  
E555

S561  
F562

V565  
H566  
R567

V577  
K578  
L579

E582

GLN  
ASP  
PHE  
HIS  
A587  
E588  
R589  
V590  
H591  
E592

Chain B:

2% 65% 20% 14%

Amino Acid	Frequency (%)
MET	2%
LYS	0%
HIS	0%
HIS	0%
HIS	0%
HIS	0%
HIS	0%
PRO	0%
MET	0%
SER	0%
ASP	0%
TYR	0%
ASP	0%
ILE	0%
PRO	0%
THR	0%
THR	0%
GLU	0%
ASN	0%
LEU	0%
PHE	0%
GLY	0%
GLY	0%
ALA	0%
MET	0%
D540	0%
D543	0%
K556	0%
A559	0%
GLY	0%
SER	0%
PHE	0%
GLY	0%
T564	0%
L579	0%
D584	0%
R589	0%
V590	0%
F593	0%
A598	0%
R602	0%
R604	0%
H605	0%
P606	0%
N607	0%
F611	0%

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.27Å 95.27Å 179.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.20 – 2.99 46.05 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.3 (46.20-2.99) 98.4 (46.05-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.201 , 0.256 0.213 , 0.254	Depositor DCC
$R_{free}$ test set	882 reflections (5.45%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.3	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 17072 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4319	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, STU, SEP

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	0.27	0/2147	0.40	0/2905
1	B	0.26	0/2168	0.40	0/2933
All	All	0.26	0/4315	0.40	0/5838

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2132	0	2134	66	0
1	B	2152	0	2155	50	0
2	A	35	0	26	6	0
All	All	4319	0	4315	117	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 14.

The worst 5 of 117 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:706:LEU:HD13	1:B:728:SER:O	1.71	0.89
2:A:1:STU:H16	2:A:1:STU:H261	1.58	0.84
1:A:554:LYS:HB3	1:A:555:GLU:OE1	1.77	0.84
1:A:554:LYS:HB2	1:A:567:ARG:O	1.85	0.77
1:A:619:PRO:HD2	1:A:620:ASN:OD1	1.85	0.77

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	260/309 (84%)	248 (95%)	12 (5%)	0	100	100
1	B	260/309 (84%)	246 (95%)	14 (5%)	0	100	100
All	All	520/618 (84%)	494 (95%)	26 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	227/268 (85%)	226 (100%)	1 (0%)	93	98
1	B	231/268 (86%)	228 (99%)	3 (1%)	76	93
All	All	458/536 (85%)	454 (99%)	4 (1%)	84	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	620	ASN
1	B	668	ARG
1	B	694	ASP
1	B	709	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	645	GLN
1	B	674	HIS
1	B	605	HIS
1	A	605	HIS
1	B	645	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	704	1	8,10,11	1.09	0	7,14,16	0.98	0
1	SEP	A	707	1	8,9,10	1.32	1 (12%)	8,12,14	2.80	3 (37%)
1	SEP	A	710	1	8,9,10	1.26	1 (12%)	8,12,14	1.47	1 (12%)
1	TPO	B	704	1	8,10,11	1.13	0	7,14,16	1.22	1 (14%)
1	SEP	B	707	1	8,9,10	1.52	1 (12%)	8,12,14	1.40	1 (12%)
1	SEP	B	710	1	8,9,10	1.52	1 (12%)	8,12,14	1.55	1 (12%)

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	704	1	-	0/8/11/13	0/0/0/0
1	SEP	A	707	1	-	0/6/8/10	0/0/0/0
1	SEP	A	710	1	-	0/6/8/10	0/0/0/0
1	TPO	B	704	1	-	0/8/11/13	0/0/0/0
1	SEP	B	707	1	-	0/6/8/10	0/0/0/0
1	SEP	B	710	1	-	0/6/8/10	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	710	SEP	P-O1P	2.62	1.59	1.51
1	A	707	SEP	P-O1P	2.75	1.60	1.51
1	B	707	SEP	P-O1P	3.11	1.61	1.51
1	B	710	SEP	P-O1P	3.13	1.61	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	707	SEP	O-C-CA	-2.24	119.66	125.49
1	B	704	TPO	CG2-CB-CA	-2.07	108.97	113.17
1	A	707	SEP	OG-P-O1P	2.20	112.73	107.14
1	B	707	SEP	OG-CB-CA	2.95	110.79	108.27
1	A	710	SEP	OG-CB-CA	3.20	111.00	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	710	SEP	3	0
1	B	704	TPO	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

1 ligand is 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	STU	A	1	-	27,42,42	0.87	0	23,68,68	1.53	5 (21%)

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	STU	A	1	-	-	0/4/42/42	0/0/8/8

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	STU	C27-O6-C22	-4.48	105.82	114.39
2	A	1	STU	C14-C13-C12	-2.25	116.92	120.79
2	A	1	STU	C3-C4-C5	-2.20	116.99	120.79
2	A	1	STU	O5-C8-C7	-2.17	124.99	128.62
2	A	1	STU	C13-C12-C17	2.28	122.27	119.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	STU	6	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	264/309 (85%)	0.08	7 (2%) 58 28	19, 51, 125, 215	0
1	B	264/309 (85%)	-0.03	6 (2%) 64 33	25, 52, 112, 168	0
All	All	528/618 (85%)	0.03	13 (2%) 61 30	19, 52, 120, 215	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	711	ALA	4.5
1	A	582	GLU	4.2
1	A	590	VAL	4.1
1	B	712	ALA	3.7
1	A	562	PHE	2.8

### 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. 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	A	704	11/12	0.89	0.24	-	69,90,102,102	0
1	TPO	B	704	11/12	0.96	0.19	-	60,88,99,100	0
1	SEP	B	710	10/11	0.78	0.34	-	121,127,189,190	0
1	SEP	A	710	10/11	0.78	0.22	-	125,127,139,140	0
1	SEP	B	707	10/11	0.71	0.32	-	156,161,164,164	0
1	SEP	A	707	10/11	0.83	0.19	-	118,143,149,151	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
2	STU	A	1	35/35	0.93	0.29	1.29	73,73,73,73	35

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

There are no such residues in this entry.