



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 01:55 PM GMT

PDB ID : 2GCD  
Title : TAO2 kinase domain-staurosporine structure  
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Deposited on : 2006-03-14  
Resolution : 2.55 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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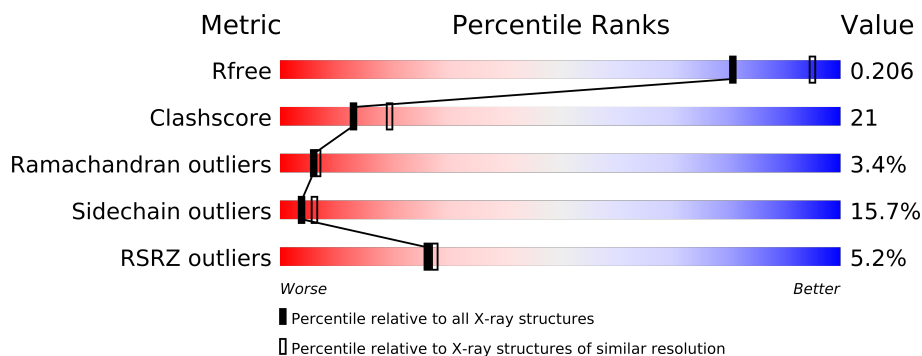
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
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)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.55 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	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

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	309	
1	B	309	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5327 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.

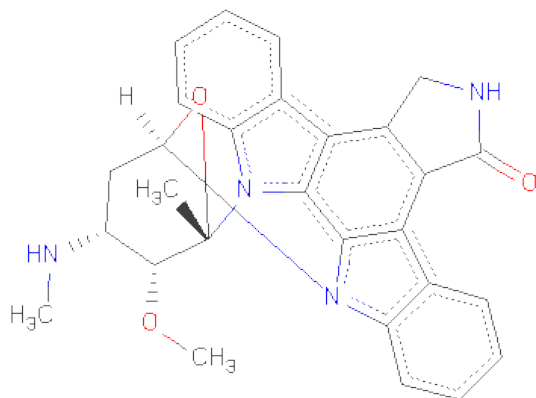
- Molecule 1 is a protein called Serine/threonine-proteinkinase TAO2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	P	S	0	0	0
			2490	1586	432	457	1	14			
1	B	309	Total	C	N	O	P	S	0	0	0
			2490	1586	432	457	1	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	SEP	SER	MODIFIED RESIDUE	UNP Q9JLS3
B	181	SEP	SER	MODIFIED RESIDUE	UNP Q9JLS3

- 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		

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

- Molecule 3 is water.

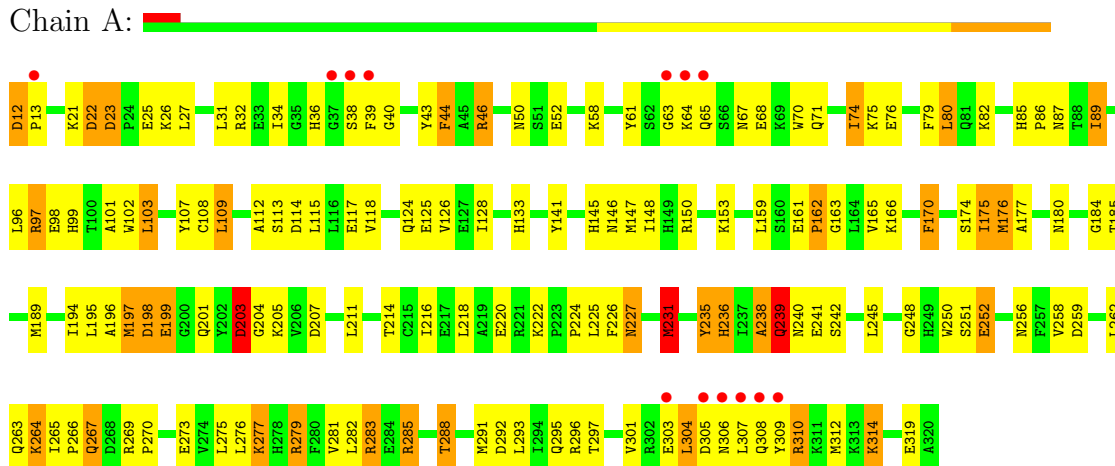
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	135	Total	O	0	0
			135	135		

### 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.

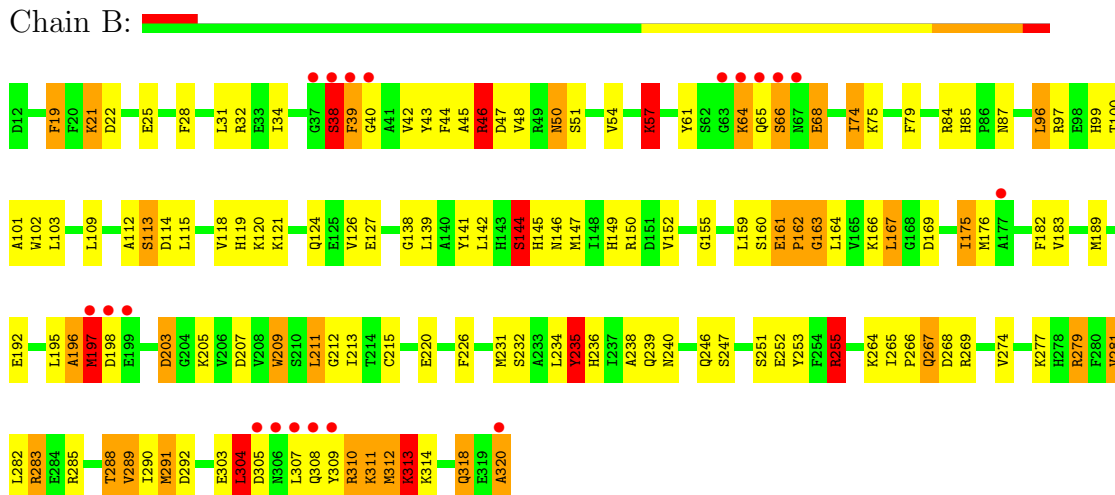
#### • Molecule 1: Serine/threonine-proteinkinase TAO2

Chain A:



#### • Molecule 1: Serine/threonine-proteinkinase TAO2

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.02Å 186.02Å 94.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	160.13 – 2.55 24.89 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.8 (160.13-2.55) 92.3 (24.89-2.55)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.53Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.199 , 0.261 0.198 , 0.206	Depositor DCC
$R_{free}$ test set	1456 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.1	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 31260 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5327	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: 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	1.58	21/2538 (0.8%)	1.38	24/3428 (0.7%)
1	B	1.57	19/2538 (0.7%)	1.37	16/3428 (0.5%)
All	All	1.58	40/5076 (0.8%)	1.37	40/6856 (0.6%)

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	1
1	B	0	2
All	All	0	3

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	GLU	CG-CD	12.50	1.70	1.51
1	A	98	GLU	CG-CD	9.10	1.65	1.51
1	A	68	GLU	CB-CG	8.90	1.69	1.52
1	B	192	GLU	CB-CG	-8.76	1.35	1.52
1	A	199	GLU	CG-CD	8.49	1.64	1.51

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ASP	CB-CG-OD2	8.70	126.13	118.30
1	A	89	ILE	CG1-CB-CG2	-7.95	93.91	111.40
1	A	207	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	32	ARG	NE-CZ-NH2	-7.41	116.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	LYS	CD-CE-NZ	7.18	128.21	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	197	MET	Peptide
1	B	196	ALA	Peptide
1	B	313	LYS	Peptide

## 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	2490	0	2468	107	0
1	B	2490	0	2468	91	0
2	A	35	0	26	3	0
2	B	35	0	26	7	0
3	A	142	0	0	14	0
3	B	135	0	0	6	0
All	All	5327	0	4988	207	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 21.

The worst 5 of 207 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:175:ILE:CG1	1:A:175:ILE:CD1	1.74	1.58
2:B:500:STU:H261	2:B:500:STU:H16	1.23	1.10
1:A:65:GLN:HE21	1:A:67:ASN:HB2	1.16	1.08
1:A:65:GLN:NE2	1:A:67:ASN:HB2	1.73	1.02
1:B:46:ARG:HH11	1:B:46:ARG:HG2	1.25	0.98

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	306/309 (99%)	269 (88%)	26 (8%)	11 (4%)	5	6
1	B	306/309 (99%)	266 (87%)	30 (10%)	10 (3%)	6	7
All	All	612/618 (99%)	535 (87%)	56 (9%)	21 (3%)	6	7

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	251	SER
1	B	39	PHE
1	B	64	LYS
1	B	162	PRO

### 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	268/268 (100%)	228 (85%)	40 (15%)	4	7
1	B	268/268 (100%)	224 (84%)	44 (16%)	3	5
All	All	536/536 (100%)	452 (84%)	84 (16%)	4	6

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	ASP
1	B	57	LYS
1	B	304	LEU
1	A	310	ARG

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Mol	Chain	Res	Type
1	B	25	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	HIS
1	A	146	ASN
1	A	236	HIS
1	A	133	HIS
1	A	227	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	SEP	A	181	1	9,9,10	8.75	4 (44%)	10,12,14	2.92	4 (40%)
1	SEP	B	181	1	9,9,10	5.84	4 (44%)	10,12,14	3.10	6 (60%)

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	SEP	A	181	1	-	0/6/8/10	0/0/0/0
1	SEP	B	181	1	-	0/6/8/10	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	SEP	O-C	25.70	1.29	1.11
1	B	181	SEP	O-C	16.79	1.22	1.11
1	A	181	SEP	P-O1P	3.59	1.63	1.51
1	A	181	SEP	CA-C	2.90	1.53	1.48
1	B	181	SEP	P-O1P	2.53	1.59	1.51

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	SEP	O3P-P-OG	-6.17	89.63	106.65
1	B	181	SEP	O2P-P-OG	-5.41	91.72	106.65
1	B	181	SEP	O3P-P-O2P	5.33	128.38	107.61
1	A	181	SEP	C-CA-N	-4.54	109.30	113.83
1	A	181	SEP	O3P-P-O1P	3.48	121.82	110.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	STU	A	400	-	40,42,42	1.63	11 (27%)	62,68,68	2.32	21 (33%)
2	STU	B	500	-	40,42,42	3.04	19 (47%)	62,68,68	2.62	23 (37%)

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	400	-	-	0/4/42/42	0/0/8/8
2	STU	B	500	-	-	0/4/42/42	0/0/8/8

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	STU	C3-C4	6.55	1.51	1.36
2	B	500	STU	C19-N3	-5.83	1.31	1.39
2	B	500	STU	C13-C12	5.82	1.53	1.40
2	B	500	STU	C15-C16	5.77	1.49	1.36
2	B	500	STU	C17-N2	-5.13	1.32	1.39

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	STU	C28-N4-C23	-9.62	108.46	113.82
2	B	500	STU	O5-C8-N1	7.34	135.81	125.50
2	B	500	STU	O5-C8-C7	-6.27	115.80	128.53
2	B	500	STU	C26-C21-C22	-6.08	98.40	112.87
2	B	500	STU	C24-C25-N3	5.84	119.19	112.48

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	309/309 (100%)	-0.02	13 (4%) 35 37	15, 37, 83, 117	0
1	B	309/309 (100%)	0.03	19 (6%) 21 21	16, 37, 84, 113	0
All	All	618/618 (100%)	0.01	32 (5%) 26 27	15, 37, 84, 117	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	TYR	9.0
1	A	63	GLY	6.9
1	A	309	TYR	6.6
1	B	308	GLN	6.4
1	A	305	ASP	5.0

### 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	B	181	10/11	0.08	-0.84	33,37,41,43	0
1	SEP	A	181	10/11	0.09	-0.86	36,37,40,46	0

### 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	STU	B	500	35/35	0.11	-0.25	18,22,24,29	0
2	STU	A	400	35/35	0.10	-0.61	27,29,34,40	0

## 6.5 Other polymers

There are no such residues in this entry.