



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 06:51 pm GMT

PDB ID : 1KFE  
Title : CRYSTAL STRUCTURE OF ALPHAT183V MUTANT OF TRYPTOPHAN SYNTHASE FROM SALMONELLA TYPHIMURIUM WITH L-Ser Bound To The Beta Site  
Authors : Kulik, V.; Weyand, M.; Siedel, R.; Niks, D.; Arac, D.; Dunn, M.F.; Schlichting, I.  
Deposited on : 2001-11-20  
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure 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

<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	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

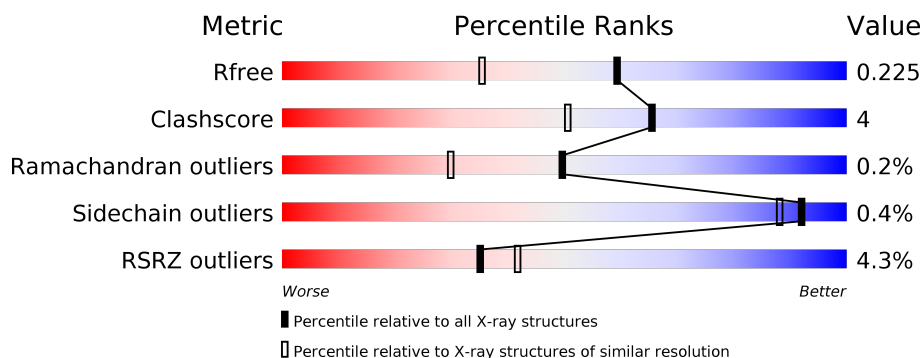
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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))
$R_{free}$	111664	1952 (1.76-1.76)
Clashscore	122126	2072 (1.76-1.76)
Ramachandran outliers	120053	2050 (1.76-1.76)
Sidechain outliers	120020	2050 (1.76-1.76)
RSRZ outliers	108989	1913 (1.76-1.76)

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	268	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>6%</div> </div> </div>
2	B	394	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5386 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 TRYPTOPHAN SYNTHASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			1890	1201	325	356	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	ILE	LEU	CLONING ARTIFACT	UNP P00929
A	183	VAL	THR	ENGINEERED	UNP P00929

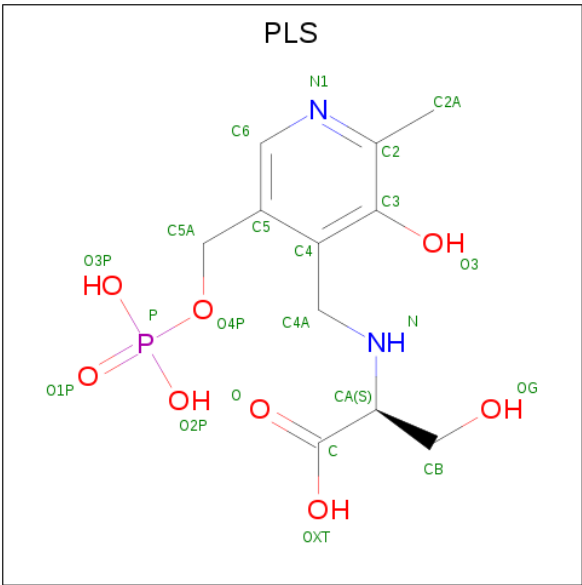
- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	394	Total	C	N	O	S	0	0	0
			2967	1864	519	565	19			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is [3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL METHYL]-SERINE (three-letter code: PLS) (formula: C<sub>11</sub>H<sub>17</sub>N<sub>2</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			22	11	2	8	1		

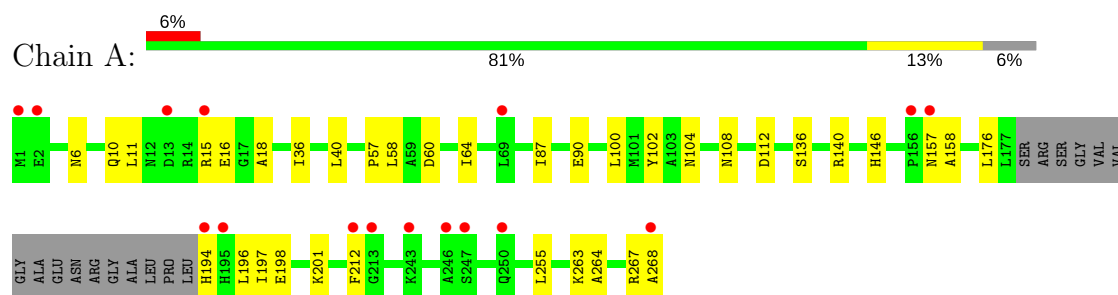
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	181	Total	O	0	0
			181	181		
5	B	325	Total	O	0	0
			325	325		

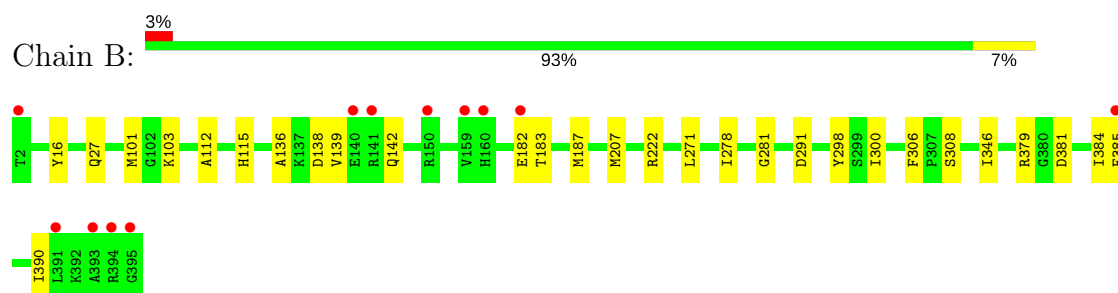
### 3 Residue-property plots [i](#)

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: TRYPTOPHAN SYNTHASE ALPHA CHAIN



#### • Molecule 2: TRYPTOPHAN SYNTHASE BETA CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.22Å 59.98Å 67.07Å 90.00° 94.68° 90.00°	Depositor
Resolution (Å)	19.97 – 1.75 23.81 – 1.74	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.97-1.75) 94.5 (23.81-1.74)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 1.74Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.192 , 0.225 0.192 , 0.225	Depositor DCC
$R_{free}$ test set	3542 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.7	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 52.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5386	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% 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: NA, PLS

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	0.42	0/1926	0.66	0/2618
2	B	0.50	0/3025	0.71	0/4090
All	All	0.47	0/4951	0.69	0/6708

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	298	TYR	Sidechain

### 5.2 Too-close contacts [i](#)

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	1890	0	1881	23	0
2	B	2967	0	2926	21	0
3	B	1	0	0	0	0
4	B	22	0	14	0	0
5	A	181	0	0	6	0
5	B	325	0	0	2	0
All	All	5386	0	4821	43	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 4.

All (43) 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:194:HIS:O	1:A:198:GLU:HG2	1.83	0.78
1:A:90:GLU:HG3	5:A:449:HOH:O	1.90	0.70
1:A:6:ASN:O	1:A:10:GLN:HG3	1.95	0.66
2:B:136:ALA:HA	2:B:139:VAL:HG12	1.78	0.66
2:B:136:ALA:HA	2:B:139:VAL:CG1	2.27	0.65
2:B:222:ARG:NH2	5:B:613:HOH:O	2.30	0.64
2:B:182:GLU:HG3	2:B:183:THR:HG23	1.79	0.63
1:A:87:ILE:HG23	5:A:333:HOH:O	2.02	0.59
1:A:100:LEU:HD21	5:A:445:HOH:O	2.03	0.57
1:A:57:PRO:HA	1:A:102:TYR:CZ	2.38	0.57
2:B:346:ILE:HG21	2:B:384:ILE:HD11	1.86	0.57
1:A:136:SER:OG	1:A:140:ARG:HD3	2.06	0.56
1:A:15:ARG:O	1:A:268:ALA:HB2	2.06	0.56
1:A:176:LEU:HD11	1:A:196:LEU:HD23	1.89	0.55
2:B:138:ASP:O	2:B:142:GLN:HB2	2.08	0.53
2:B:27:GLN:HG2	2:B:101:MET:HE3	1.91	0.53
2:B:381:ASP:HA	2:B:384:ILE:HD13	1.92	0.51
1:A:201:LYS:HA	5:A:322:HOH:O	2.10	0.51
1:A:108:ASN:HA	5:A:297:HOH:O	2.13	0.49
1:A:157:ASN:O	1:A:158:ALA:C	2.51	0.48
1:A:264:ALA:HA	1:A:267:ARG:NH1	2.28	0.48
2:B:385:PHE:HB2	5:B:778:HOH:O	2.13	0.47
1:A:58:LEU:HD12	1:A:58:LEU:C	2.35	0.47
1:A:11:LEU:CD1	1:A:18:ALA:HB2	2.44	0.47
2:B:271:LEU:O	2:B:271:LEU:HD23	2.15	0.47
1:A:36:ILE:HG23	1:A:255:LEU:HD13	1.97	0.47
1:A:36:ILE:O	1:A:40:LEU:HG	2.17	0.45
2:B:16:TYR:O	2:B:281:GLY:HA2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:ARG:HD2	2:B:381:ASP:OD1	2.17	0.45
2:B:101:MET:HE1	2:B:103:LYS:NZ	2.32	0.44
2:B:112:ALA:O	2:B:142:GLN:CG	2.66	0.44
1:A:104:ASN:HB2	2:B:278:ILE:O	2.16	0.44
1:A:197:ILE:O	1:A:201:LYS:HG3	2.18	0.44
2:B:136:ALA:O	2:B:139:VAL:HG13	2.18	0.44
2:B:271:LEU:HD23	2:B:271:LEU:C	2.38	0.43
2:B:300:ILE:HD11	2:B:390:ILE:CD1	2.49	0.43
2:B:115:HIS:HE1	2:B:187:MET:O	2.01	0.42
1:A:263:LYS:HA	1:A:263:LYS:HD2	1.94	0.42
1:A:60:ASP:HB3	1:A:64:ILE:HB	2.02	0.42
2:B:136:ALA:CA	2:B:139:VAL:HG12	2.48	0.41
1:A:112:ASP:OD1	1:A:146:HIS:HE1	2.03	0.41
1:A:16:GLU:HG3	5:A:347:HOH:O	2.21	0.40
2:B:306:PHE:CE2	2:B:308:SER:HB3	2.55	0.40

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	248/268 (92%)	241 (97%)	6 (2%)	1 (0%)	36	17
2	B	392/394 (100%)	381 (97%)	11 (3%)	0	100	100
All	All	640/662 (97%)	622 (97%)	17 (3%)	1 (0%)	49	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	PHE

### 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	193/208 (93%)	193 (100%)	0	100	100
2	B	305/308 (99%)	303 (99%)	2 (1%)	85	76
All	All	498/516 (96%)	496 (100%)	2 (0%)	92	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	207	MET
2	B	291	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	146	HIS
1	A	250	GLN
2	B	44	GLN
2	B	114	GLN
2	B	246	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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$
4	PLS	B	550	-	19,22,22	4.21	10 (52%)	25,31,31	3.38	12 (48%)

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
4	PLS	B	550	-	-	0/13/17/17	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	550	PLS	C4A-N	-4.99	1.31	1.46
4	B	550	PLS	P-O4P	-3.21	1.49	1.60
4	B	550	PLS	P-O3P	-3.00	1.42	1.54
4	B	550	PLS	P-O2P	-2.80	1.43	1.54
4	B	550	PLS	C6-N1	3.28	1.41	1.34
4	B	550	PLS	C5-C4	3.28	1.45	1.40
4	B	550	PLS	C6-C5	3.56	1.45	1.37
4	B	550	PLS	C2-N1	3.99	1.41	1.33
4	B	550	PLS	C3-C4	8.30	1.53	1.40
4	B	550	PLS	C3-C2	12.77	1.49	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	550	PLS	C5-C6-N1	-2.89	118.94	123.83
4	B	550	PLS	C3-C2-N1	-2.52	117.44	120.75
4	B	550	PLS	C4A-C4-C5	-2.26	117.12	119.71
4	B	550	PLS	C4-C3-C2	-2.03	116.89	120.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	550	PLS	C3-C4-C5	2.46	121.16	118.73
4	B	550	PLS	O4P-C5A-C5	3.67	116.45	109.39
4	B	550	PLS	C6-N1-C2	3.71	126.34	119.19
4	B	550	PLS	O3-C3-C2	4.32	126.83	117.78
4	B	550	PLS	CB-CA-N	4.52	121.01	108.91
4	B	550	PLS	O3P-P-O4P	6.99	125.34	106.73
4	B	550	PLS	C4A-N-CA	7.60	128.63	114.01
4	B	550	PLS	C4-C4A-N	8.07	133.99	111.78

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	252/268 (94%)	0.44	16 (6%)	20 26	11, 24, 42, 51	0
2	B	394/394 (100%)	0.02	12 (3%)	50 56	8, 16, 36, 59	0
All	All	646/662 (97%)	0.18	28 (4%)	35 42	8, 19, 40, 59	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	PHE	7.4
1	A	213	GLY	6.2
1	A	246	ALA	5.6
2	B	395	GLY	5.4
2	B	393	ALA	5.4
2	B	385	PHE	5.0
2	B	394	ARG	4.7
1	A	268	ALA	4.5
1	A	1	MET	3.8
1	A	157	ASN	3.7
1	A	15	ARG	3.4
2	B	182	GLU	3.3
1	A	247	SER	3.2
1	A	13	ASP	3.2
1	A	194	HIS	3.0
1	A	195	HIS	3.0
1	A	243	LYS	2.9
2	B	140	GLU	2.8
2	B	2	THR	2.8
1	A	250	GLN	2.6
2	B	391	LEU	2.6
2	B	159	VAL	2.5
1	A	156	PRO	2.4
1	A	69	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	150	ARG	2.3
1	A	2	GLU	2.3
2	B	160	HIS	2.2
2	B	141	ARG	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 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
4	PLS	B	550	22/22	0.97	0.09	12,22,24,28	0
3	NA	B	555	1/1	1.00	0.05	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.