



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:24 AM GMT

PDB ID : 3IB9
Title : Propionyl-CoA Carboxylase Beta Subunit, D422L
Authors : Diacovich, L.; Arabolaza, A.; Shillito, E.M.; Lin, T.-W.; Mitchell, D.L.; Pham, H.; Melgar, M.M.
Deposited on : 2009-07-15
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
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 (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

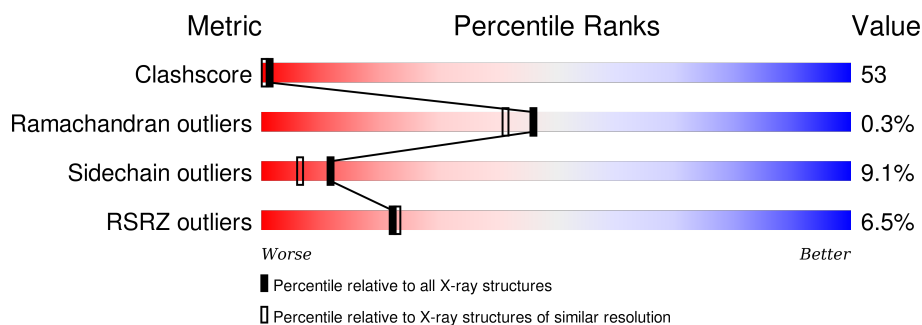
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
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 ≥ 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	530	
1	B	530	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8285 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.

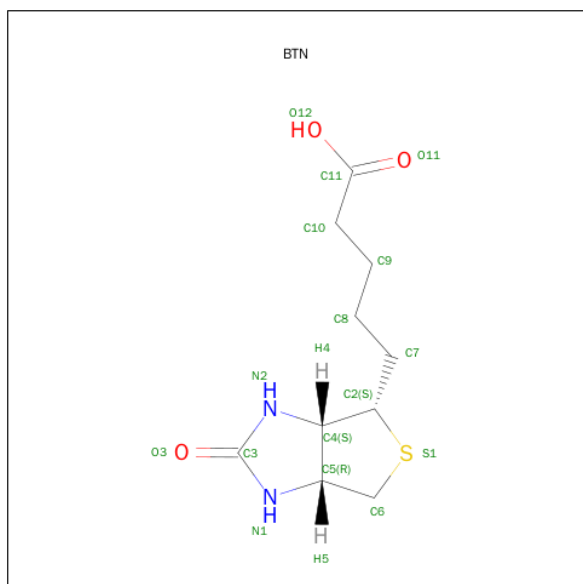
- Molecule 1 is a protein called Propionyl-CoA carboxylase complex B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			3952	2483	698	758	13			
1	B	521	Total	C	N	O	S	0	0	0
			3952	2483	698	758	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	422	LEU	ASP	ENGINEERED	UNP Q9X4K7
B	422	LEU	ASP	ENGINEERED	UNP Q9X4K7

- Molecule 2 is BIOTIN (three-letter code: BTN) (formula: C₁₀H₁₆N₂O₃S).



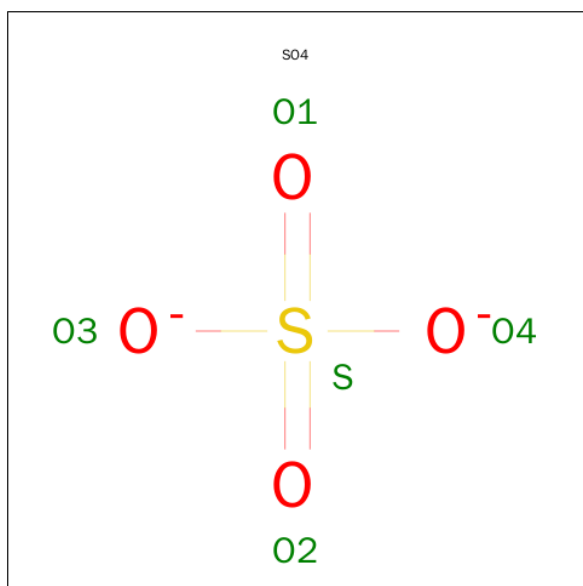
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			16	10	2	3	1		

- Molecule 3 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

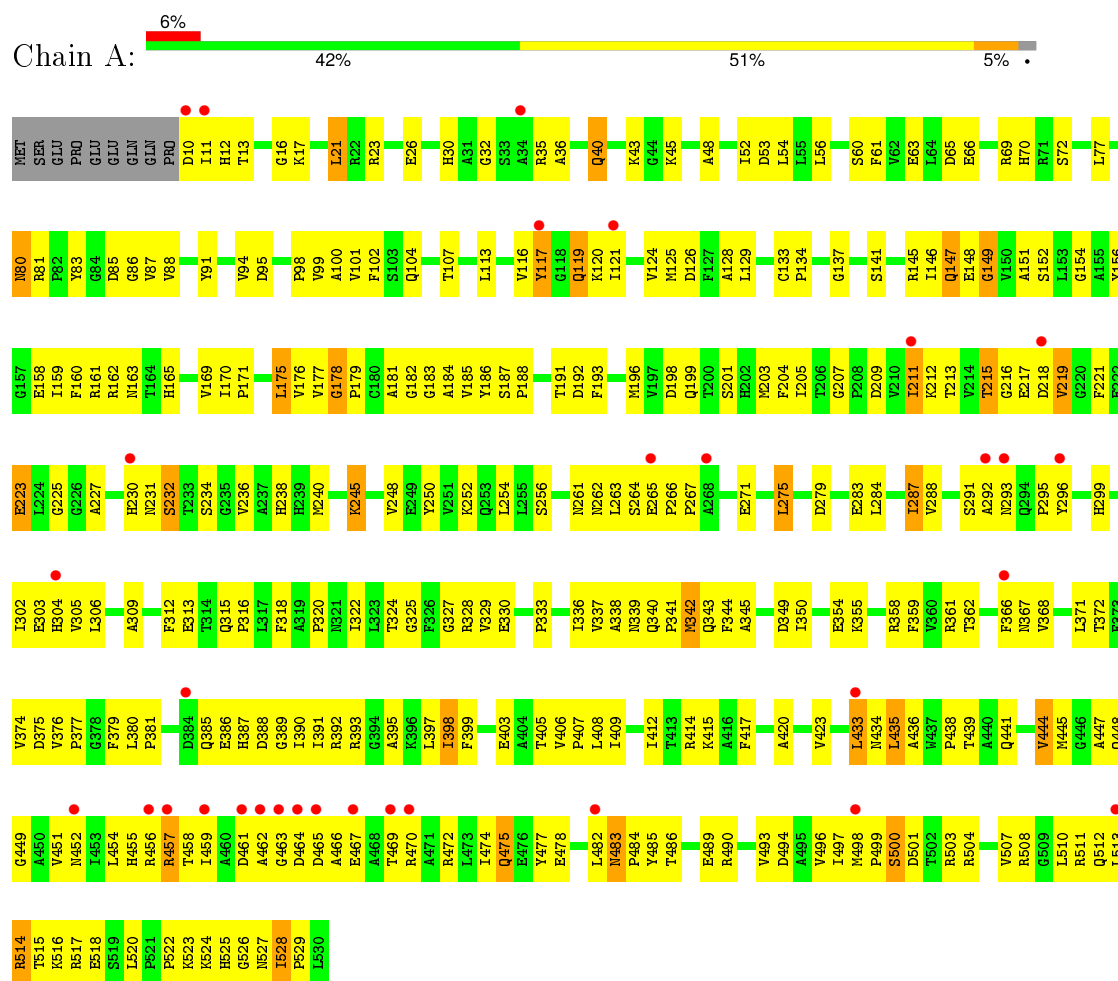
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	167	Total	O	0	0
			167	167		
4	B	172	Total	O	0	0
			172	172		

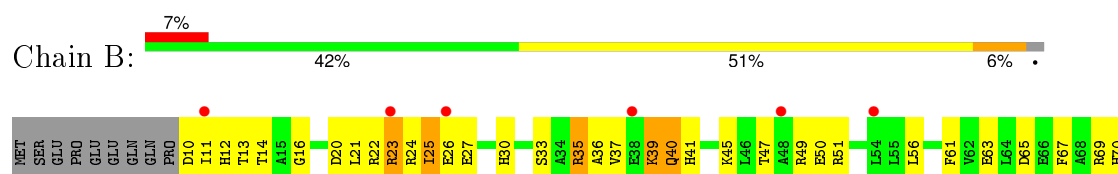
3 Residue-property plots

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: Propionyl-CoA carboxylase complex B subunit



- Molecule 1: Propionyl-CoA carboxylase complex B subunit



R504	M434	C363	K292	V136	R71
H505	L435	D364	K212	G137	S72
I506	A436		T213		
V507	M437		V214	D140	F75
R508	P438		T215	S141	G76
G509	T439		D218	G142	L77
	A440		V219	G143	D78
L513	Q441		G220	T146	A79
R514	I442		F221	Q147	N80
	A443			E148	R81
L520	V444		G226		P82
P521	M445		A227	L153	Y83
P522	G446		R228		G84
K523	A447		T229	Y156	D85
	Q448		N231	G157	G86
I528	G449		E232	E158	V87
P529	A450		I159	F160	
L530	V451		T233	R161	Y91
			S234	A162	
	L454		V235	N163	Y94
	H455		V236	T164	D95
	R456		H238	A165	G96
	R457		E239	A166	R97
	T458		R240		P98
	I459		A241	V169	Y99
	A460		K245	I170	A100
	D461		I173		I101
	A462		A247	V177	F102
	G463		V251	C180	S103
	D464		Q252	A181	G104
	D465		Q253	G182	D105
	A466		L254	G183	F106
	E467		L255	A184	
	A468		S256	V185	G114
	A469		T257	Y186	E115
	A470		N261	P187	V116
	A471		E265	A189	Y117
	R472		P266	I190	G118
L473	L474		T267	T191	Q119
I474	Q475		A268	D192	K120
Q475	E476		F269	F193	I121
E476	Y477		T194	T194	V122
Y477	E478		E271	V195	K123
			V277	D198	V124
	L482		E280	Q199	M125
	N483		L348	T200	D126
P484	P484		Q343	F204	F127
Y485	G419		A345	I205	A128
	E489		G346	T206	L129
	M424		C347	G207	K130
V493	G425		D349	G208	G132
D494	K427		I350	P208	P134
	H428		K355		V135
I497	L429		R358		
	D501		F359		
T502	G430				
R503	L433				

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	168.49 Å 168.49 Å 80.31 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.00 29.60 – 1.90	Depositor EDS
% Data completeness (in resolution range)	75.7 (50.00-2.00) 70.8 (29.60-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.86 (at 1.89 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.274 0.302 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 31.2	EDS
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	10 of 91097 reflections (0.011%)	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	8285	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: BTN, SO4

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	0.23	0/4032	0.49	2/5478 (0.0%)
1	B	0.24	0/4032	0.49	0/5478
All	All	0.24	0/8064	0.49	2/10956 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	GLY	C-N-CD	-5.88	107.67	120.60
1	A	149	GLY	N-CA-C	5.04	125.69	113.10

There are no chirality outliers.

There are no planarity outliers.

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	3952	0	3887	461	0
1	B	3952	0	3887	432	0
2	A	16	0	15	2	0
2	B	16	0	15	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	167	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	172	0	0	13	0
All	All	8285	0	7804	842	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 53.

The worst 5 of 842 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:87:VAL:HB	1:A:117:TYR:CE2	1.33	1.57
1:A:456:ARG:NH1	1:A:457:ARG:HH22	1.30	1.29
1:A:87:VAL:HB	1:A:117:TYR:CD2	1.68	1.26
1:B:113:LEU:HD13	1:B:156:TYR:CE1	1.72	1.25
1:A:456:ARG:NH1	1:A:457:ARG:NH2	1.91	1.18

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	519/530 (98%)	459 (88%)	58 (11%)	2 (0%)	39	33
1	B	519/530 (98%)	458 (88%)	60 (12%)	1 (0%)	52	48
All	All	1038/1060 (98%)	917 (88%)	118 (11%)	3 (0%)	46	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	463	GLY
1	A	514	ARG
1	B	98	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	412/421 (98%)	374 (91%)	38 (9%)	11	6
1	B	412/421 (98%)	375 (91%)	37 (9%)	12	7
All	All	824/842 (98%)	749 (91%)	75 (9%)	12	6

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	475	GLN
1	B	39	LYS
1	B	458	THR
1	A	483	ASN
1	B	23	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	483	ASN
1	A	527	ASN
1	B	483	ASN
1	A	505	HIS
1	B	30	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	SO4	A	531	-	4,4,4	0.22	0	6,6,6	0.12	0
2	BTN	A	5600	-	12,17,17	4.66	8 (66%)	13,23,23	4.00	6 (46%)
3	SO4	B	531	-	4,4,4	0.19	0	6,6,6	0.13	0
2	BTN	B	5601	-	12,17,17	4.28	8 (66%)	13,23,23	4.37	5 (38%)

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	SO4	A	531	-	-	0/0/0/0	0/0/0/0
2	BTN	A	5600	-	-	0/5/28/28	0/2/2/2
3	SO4	B	531	-	-	0/0/0/0	0/0/0/0
2	BTN	B	5601	-	-	0/5/28/28	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5600	BTN	C3-N1	-5.88	1.27	1.35
2	B	5601	BTN	C3-N1	-5.67	1.27	1.35
2	B	5601	BTN	C5-C4	-3.07	1.51	1.56
2	A	5600	BTN	C5-C4	-3.04	1.51	1.56
2	B	5601	BTN	O3-C3	2.79	1.29	1.23

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5601	BTN	O3-C3-N2	-9.51	114.86	125.90
2	A	5600	BTN	O3-C3-N2	-8.29	116.28	125.90
2	B	5601	BTN	C4-N2-C3	-7.96	105.05	112.66
2	A	5600	BTN	C4-N2-C3	-7.60	105.39	112.66
2	A	5600	BTN	C7-C2-S1	2.11	117.36	112.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5600	BTN	2	0
2	B	5601	BTN	2	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, 95th 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 ²)	Q<0.9
1	A	521/530 (98%)	0.50	32 (6%) 25 26	22, 30, 55, 113	0
1	B	521/530 (98%)	0.54	36 (6%) 20 21	22, 31, 56, 102	0
All	All	1042/1060 (98%)	0.52	68 (6%) 22 23	22, 30, 56, 113	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	462	ALA	6.3
1	B	464	ASP	6.1
1	B	462	ALA	5.3
1	A	463	GLY	5.2
1	A	465	ASP	4.6

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. 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, 95th 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(\AA^2)	Q<0.9
2	BTN	A	5600	16/16	0.85	0.16	0.59	54,57,69,70	0
2	BTN	B	5601	16/16	0.78	0.19	0.56	55,58,75,75	0
3	SO4	A	531	5/5	0.96	0.15	-0.08	38,38,39,41	0
3	SO4	B	531	5/5	0.98	0.12	-0.33	36,38,39,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.