



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 05:41 PM UTC

PDB ID : 3IB9 / pdb_00003ib9
Title : Propionyl-CoA Carboxylase Beta Subunit, D422L
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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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

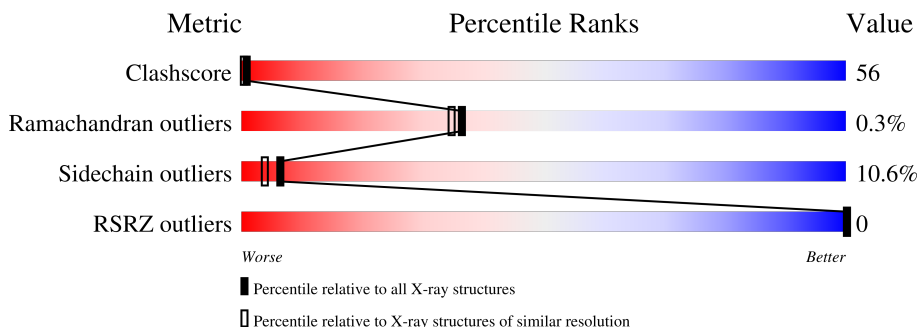
1 Overall quality at a glance

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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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.

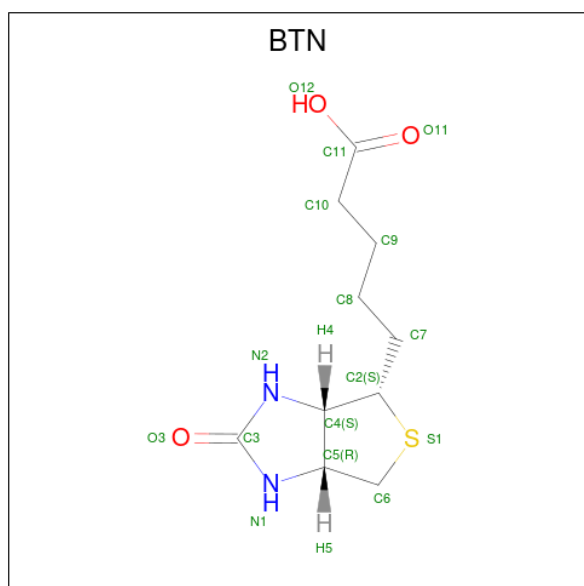
- Molecule 1 is a protein called Propionyl-CoA carboxylase complex B subunit.

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 mutation	UNP Q9X4K7
B	422	LEU	ASP	engineered mutation	UNP Q9X4K7

- Molecule 2 is BIOTIN (CCD ID: BTN) (formula: $C_{10}H_{16}N_2O_3S$).



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 (CCD ID: 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		

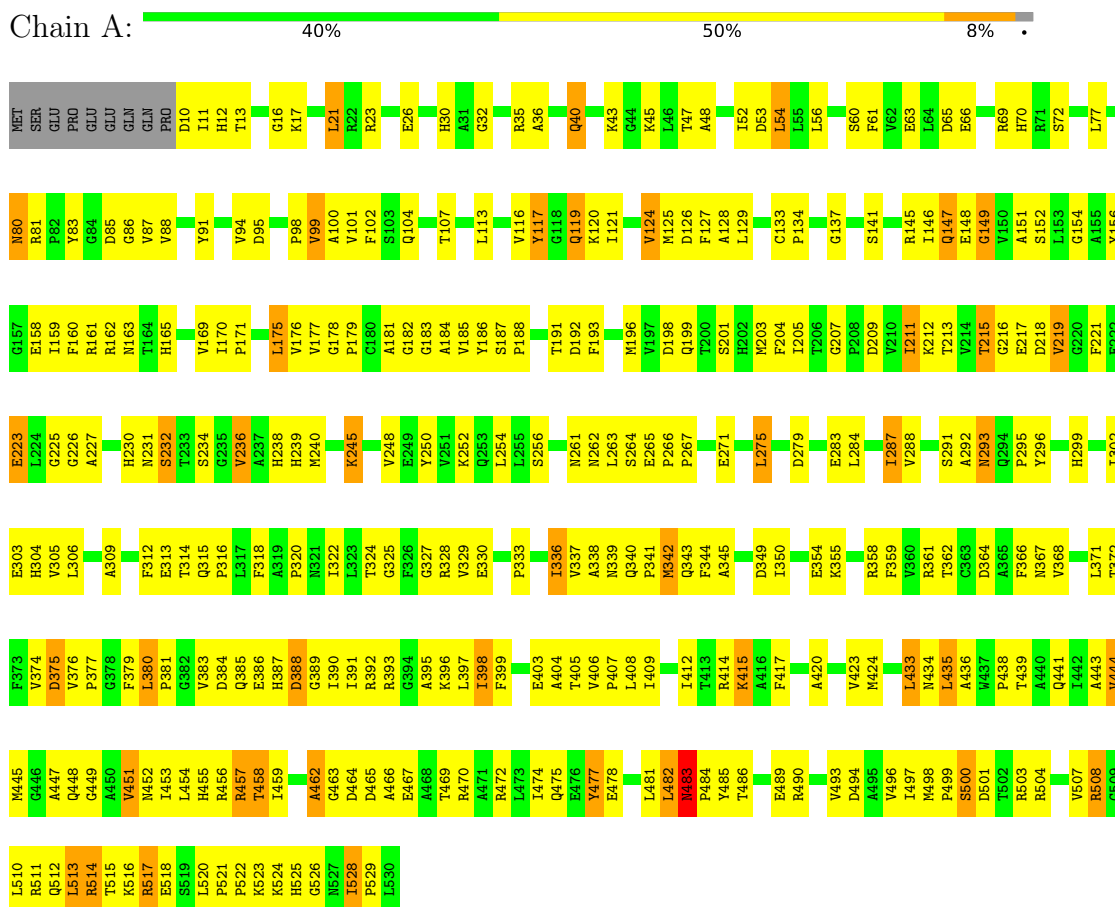
- Molecule 4 is water.

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

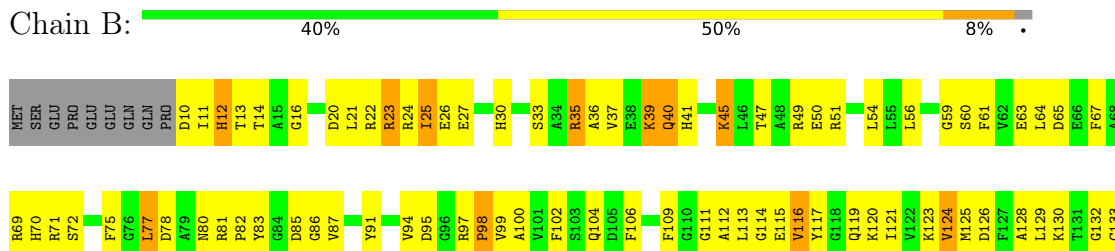
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Propionyl-CoA carboxylase complex B subunit



• Molecule 1: Propionyl-CoA carboxylase complex B subunit



D501	L433	R358	V288	G207	P134
T502	L434	F359	N293	P208	V135
R503	L435	C363	N294	K212	V136
R504	A436	D364	P295	T213	G137
H505	W437	N367	D297	Y214	D140
I506	P438	V368	M298	T215	S141
V507	T439	L371	H299	V219	G142
R508	A440		S300	G220	G143
G509	Q441		V301	F221	I146
L513	I442	V374	I302	G226	Q147
R514	A443	D375	F303	A227	E148
	W444	V376	H304	R228	
L520	M445	P377	V305	T229	L153
P521	G446	G378	L306	H230	G154
P522	A447	F379	D307	N231	A155
K523	Q448	L380	D308	H232	Y156
	Q449	P381	A309	S232	G157
I528	A450	H387	E310	T233	E158
P529	V451		F311	S234	I159
L530		I390	F312	G235	F160
	L454	I391	E313	V236	R161
	H455	R392	T314	A237	R162
	R456	R393	Q315	H238	N163
	R457	G394	P316	H239	T164
	T458	A395	L317	M240	H165
	I459	R396	A319	A241	A166
	A460	L397	F318		
	A461	I398	P320	K245	V169
	A462	F399	N321	D246	I170
	G463	A400	I322	A247	
	D464	Y401	L323	V251	I173
	D465	A402	T324	K252	V177
	A466	E403	F326	Q253	
	A468	A404	G327	L254	G180
	T469	T405	R328	L255	A181
	R470	V406	V329	S256	G182
	A471	P407	E330	Y257	G183
	R472	L408	G331		A184
	L473	I409	R332	N261	V185
	I474		I336	E265	Y186
	Q475	I412		P266	S187
	E476	T413	N339	P267	P188
	Y477	R414	Q340	A268	A189
	E478	K415	P341	F269	I190
		A416	M342	P270	T191
	L482	F417	Q343	E271	D192
	M483	G418	F344		F193
	P484	Q419	A345	V277	T194
	Y485		G346	E280	V195
	T486	V423	C347	D281	
		M424	I348	A282	D198
	E489	G425	D349	I350	Q199
		S426	K355		T200
	V493	K427		E283	
	D494	L429		L284	F204
		I497		I287	I205
					T206

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	168.49Å 168.49Å 80.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	75.7 (50.00-2.00) 75.7 (50.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-3.70 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.246 , 0.274 0.315 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	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 14.06% 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, 0.333 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: 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	0.32	0/4032	0.82	11/5478 (0.2%)
1	B	0.34	1/4032 (0.0%)	0.85	14/5478 (0.3%)
All	All	0.33	1/8064 (0.0%)	0.84	25/10956 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	155	ALA	C-N	5.44	1.40	1.33

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	VAL	N-CA-C	10.81	120.69	110.53
1	B	463	GLY	N-CA-C	-7.95	105.57	114.40
1	B	12	HIS	CA-C-N	7.64	133.27	122.72
1	B	12	HIS	C-N-CA	7.64	133.27	122.72
1	A	388	ASP	N-CA-C	-7.43	103.17	111.71

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	482	0
1	B	3952	0	3887	449	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
4	B	172	0	0	13	0
All	All	8285	0	7804	878	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 56.

The worst 5 of 878 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%)	30	27
1	B	519/530 (98%)	458 (88%)	60 (12%)	1 (0%)	43	42
All	All	1038/1060 (98%)	917 (88%)	118 (11%)	3 (0%)	36	35

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 [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	412/421 (98%)	364 (88%)	48 (12%)	5	3
1	B	412/421 (98%)	373 (90%)	39 (10%)	8	5
All	All	824/842 (98%)	737 (89%)	87 (11%)	6	4

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	77	LEU
1	B	280	GLU
1	B	146	ILE
1	B	212	LYS
1	B	398	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	339	ASN
1	B	441	GLN
1	B	505	HIS
1	A	448	GLN
1	A	385	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	B	531	-	4,4,4	0.32	0	6,6,6	0.14	0
3	SO4	A	531	-	4,4,4	0.36	0	6,6,6	0.16	0
2	BTN	A	5600	-	17,17,17	3.77	8 (47%)	23,23,23	2.79	7 (30%)
2	BTN	B	5601	-	17,17,17	3.44	7 (41%)	23,23,23	2.96	7 (30%)

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	BTN	A	5600	-	-	4/7/28/28	0/2/2/2
2	BTN	B	5601	-	-	4/7/28/28	0/2/2/2

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5600	BTN	C5-N1	8.23	1.58	1.46
2	B	5601	BTN	C5-N1	6.94	1.56	1.46
2	A	5600	BTN	C2-S1	6.80	1.93	1.82
2	B	5601	BTN	C2-S1	6.62	1.93	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5600	BTN	C3-N2	6.06	1.46	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5601	BTN	O3-C3-N2	-7.67	114.86	125.89
2	A	5600	BTN	O3-C3-N2	-6.68	116.28	125.89
2	B	5601	BTN	C4-N2-C3	-6.05	105.05	112.56
2	A	5600	BTN	C4-N2-C3	-5.77	105.39	112.56
2	A	5600	BTN	C6-C5-N1	-5.50	106.10	113.18

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5600	BTN	C7-C8-C9-C10
2	B	5601	BTN	C11-C10-C9-C8
2	A	5600	BTN	C11-C10-C9-C8
2	B	5601	BTN	C7-C8-C9-C10
2	B	5601	BTN	C9-C10-C11-O12

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%)	-1.29	0 100 100	22, 30, 54, 113	0
1	B	521/530 (98%)	-1.28	0 100 100	22, 31, 56, 102	0
All	All	1042/1060 (98%)	-1.28	0 100 100	22, 30, 56, 113	0

There are no RSRZ outliers to report.

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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
2	BTN	A	5600	16/16	0.98	0.07	54,57,69,70	0
2	BTN	B	5601	16/16	0.98	0.06	55,58,75,75	0
3	SO4	B	531	5/5	0.99	0.04	36,38,39,40	0
3	SO4	A	531	5/5	1.00	0.02	38,38,39,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.