



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 07:56 PM UTC

PDB ID : 9KAU / pdb_00009kau
Title : Three-dimensional structure of homo-dimer of cystathione beta lyase/PLP/+L-alliin complex from Bacillus cereus(BcPatB)
Authors : Liu, Y.; Yang, C.
Deposited on : 2024-10-29
Resolution : 1.88 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

<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

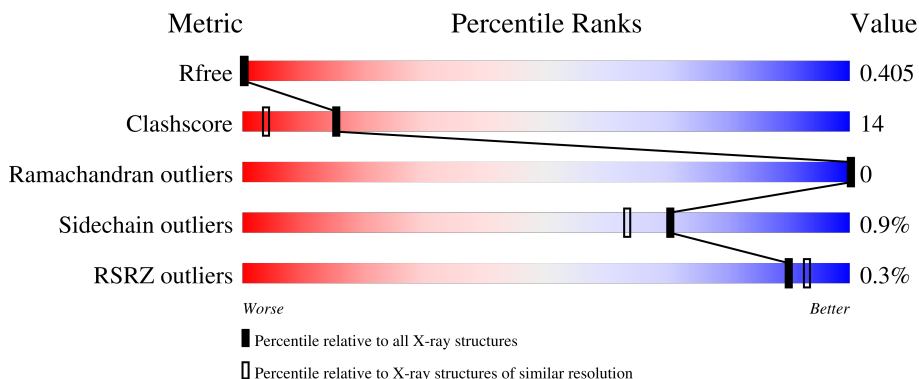
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	383	 68% 29% ..
1	B	383	 69% 27% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6217 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 cysteine-S-conjugate beta-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	P	S	0	0	0
			3058	1963	515	564	1	15			
1	B	374	Total	C	N	O	P	S	0	0	0
			3050	1961	513	560	1	15			

There are 26 discrepancies between the modelled and reference sequences:

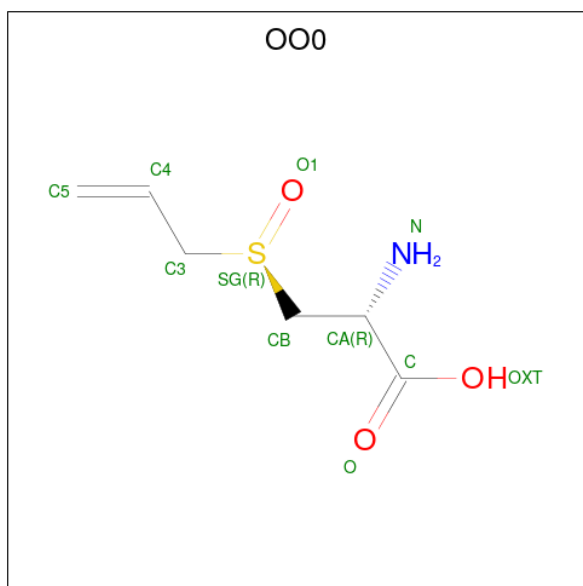
Chain	Residue	Modelled	Actual	Comment	Reference
A	51	LYS	GLU	engineered mutation	UNP A0A9X6FDP0
A	179	ILE	VAL	engineered mutation	UNP A0A9X6FDP0
A	180	LYS	GLN	engineered mutation	UNP A0A9X6FDP0
A	189	ASN	ASP	engineered mutation	UNP A0A9X6FDP0
A	286	LYS	GLU	engineered mutation	UNP A0A9X6FDP0
A	296	LYS	GLN	engineered mutation	UNP A0A9X6FDP0
A	302	MET	ILE	engineered mutation	UNP A0A9X6FDP0
A	304	ASP	THR	engineered mutation	UNP A0A9X6FDP0
A	308	THR	ALA	engineered mutation	UNP A0A9X6FDP0
A	326	ALA	ARG	engineered mutation	UNP A0A9X6FDP0
A	328	ASN	LYS	engineered mutation	UNP A0A9X6FDP0
A	332	ASP	ASN	engineered mutation	UNP A0A9X6FDP0
A	336	LYS	ALA	engineered mutation	UNP A0A9X6FDP0
B	51	LYS	GLU	engineered mutation	UNP A0A9X6FDP0
B	179	ILE	VAL	engineered mutation	UNP A0A9X6FDP0
B	180	LYS	GLN	engineered mutation	UNP A0A9X6FDP0
B	189	ASN	ASP	engineered mutation	UNP A0A9X6FDP0
B	286	LYS	GLU	engineered mutation	UNP A0A9X6FDP0
B	296	LYS	GLN	engineered mutation	UNP A0A9X6FDP0
B	302	MET	ILE	engineered mutation	UNP A0A9X6FDP0
B	304	ASP	THR	engineered mutation	UNP A0A9X6FDP0
B	308	THR	ALA	engineered mutation	UNP A0A9X6FDP0
B	326	ALA	ARG	engineered mutation	UNP A0A9X6FDP0
B	328	ASN	LYS	engineered mutation	UNP A0A9X6FDP0
B	332	ASP	ASN	engineered mutation	UNP A0A9X6FDP0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	336	LYS	ALA	engineered mutation	UNP A0A9X6FDP0

- Molecule 2 is ALLIIN (CCD ID: 000) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			11	6	1	3	1		

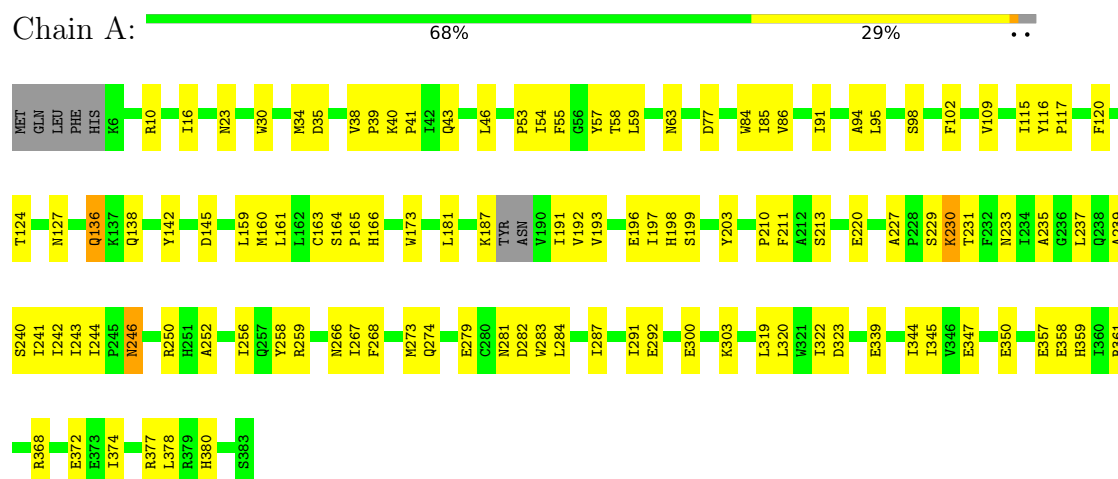
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	0
			54	54		
3	B	44	Total	O	0	0
			44	44		

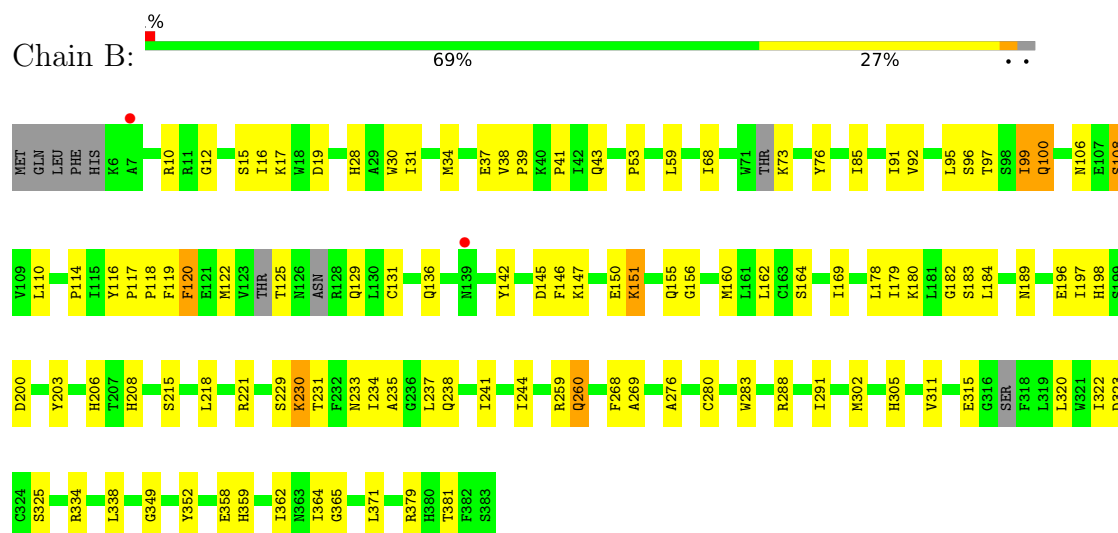
3 Residue-property plots [i](#)

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: cysteine-S-conjugate beta-lyase



• Molecule 1: cysteine-S-conjugate beta-lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.22Å 85.52Å 168.08Å 90.00° 91.12° 90.00°	Depositor
Resolution (Å)	35.46 – 1.88 35.46 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.46-1.88) 86.1 (35.46-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.16	Depositor
R, R_{free}	0.359 , 0.393 0.361 , 0.405	Depositor DCC
R_{free} test set	1993 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å ²)	10.2	Xtriage
Anisotropy	0.909	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 15.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.286 for h,-k,-l	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	6217	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: LLP, OOO

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	0.53	2/3108 (0.1%)	0.76	5/4215 (0.1%)
1	B	0.59	4/3098 (0.1%)	0.80	6/4196 (0.1%)
All	All	0.56	6/6206 (0.1%)	0.78	11/8411 (0.1%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	99	ILE	C-O	-8.28	1.14	1.24
1	B	244	ILE	C-O	-6.91	1.15	1.24
1	B	151	LYS	C-O	-6.70	1.15	1.24
1	A	377	ARG	C-O	-6.16	1.16	1.24
1	B	120	PHE	C-O	-5.23	1.17	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	260	GLN	N-CA-C	-8.12	101.05	113.89
1	A	246	ASN	CA-CB-CG	7.61	120.21	112.60
1	B	120	PHE	CA-CB-CG	6.42	120.22	113.80
1	B	99	ILE	CA-C-O	-6.41	113.94	121.05
1	B	97	THR	CA-CB-OG1	-6.21	100.29	109.60

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	3058	0	3042	91	0
1	B	3050	0	3029	85	0
2	A	11	0	0	3	0
3	A	54	0	0	13	0
3	B	44	0	0	9	0
All	All	6217	0	6071	165	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 165 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:230:LLP:H4'1	2:A:401:OO0:N	1.73	1.02
1:A:59:LEU:HG	1:B:16:ILE:HG12	1.54	0.89
1:B:85:ILE:HG23	1:B:241:ILE:HG23	1.56	0.84
1:A:292:GLU:HB2	3:A:512:HOH:O	1.81	0.80
1:A:160:MET:SD	3:A:538:HOH:O	2.40	0.79

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	371/383 (97%)	357 (96%)	14 (4%)	0	100	100
1	B	363/383 (95%)	353 (97%)	10 (3%)	0	100	100
All	All	734/766 (96%)	710 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	336/343 (98%)	335 (100%)	1 (0%)	86	82
1	B	334/343 (97%)	329 (98%)	5 (2%)	57	46
All	All	670/686 (98%)	664 (99%)	6 (1%)	70	63

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	76	TYR
1	B	100	GLN
1	B	108	SER
1	B	41	PRO
1	A	358	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	GLN
1	A	328	ASN
1	B	359	HIS
1	B	152	GLN
1	A	208	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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	LLP	A	230	1	23,24,25	1.72	5 (21%)	25,32,34	1.90	6 (24%)
1	LLP	B	230	1	23,24,25	1.78	6 (26%)	25,32,34	2.03	4 (16%)

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	LLP	A	230	1	-	6/16/17/19	0/1/1/1
1	LLP	B	230	1	-	4/16/17/19	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	LLP	C4-C4'	5.32	1.58	1.46
1	B	230	LLP	C4-C4'	5.06	1.57	1.46
1	B	230	LLP	C4'-NZ	-3.40	1.15	1.27
1	A	230	LLP	C5'-C5	2.91	1.58	1.50
1	B	230	LLP	C5'-C5	2.72	1.58	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	LLP	CE-NZ-C4'	6.89	140.79	118.72
1	A	230	LLP	OP2-P-OP4	5.40	120.74	106.67
1	B	230	LLP	C2'-C2-C3	-3.95	116.17	120.80
1	A	230	LLP	C3-C4-C4'	-3.60	113.90	120.40
1	A	230	LLP	C5-C4-C4'	3.19	126.40	121.47

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	230	LLP	C5-C4-C4'-NZ
1	A	230	LLP	C4-C4'-NZ-CE

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Mol	Chain	Res	Type	Atoms
1	A	230	LLP	C4-C5-C5'-OP4
1	A	230	LLP	C3-C4-C4'-NZ
1	B	230	LLP	C5-C4-C4'-NZ

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	230	LLP	2	0
1	B	230	LLP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	OO0	A	401	-	8,10,10	2.04	2 (25%)	5,12,12	2.13	3 (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
2	OO0	A	401	-	-	4/11/11/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	OO0	O1-SG	4.78	1.67	1.50
2	A	401	OO0	C3-C4	2.28	1.52	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	OO0	O1-SG-CB	3.15	110.35	106.12
2	A	401	OO0	OXT-C-O	-2.67	118.03	124.08
2	A	401	OO0	C4-C3-SG	-2.22	104.04	111.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	OO0	N-CA-CB-SG
2	A	401	OO0	C4-C3-SG-O1
2	A	401	OO0	C4-C3-SG-CB
2	A	401	OO0	C-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	OO0	3	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	375/383 (97%)	-0.60	0 100 100	4, 21, 39, 50	0
1	B	373/383 (97%)	-0.45	2 (0%) 87 90	2, 25, 47, 60	0
All	All	748/766 (97%)	-0.53	2 (0%) 90 93	2, 23, 44, 60	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ALA	3.2
1	B	139	ASN	3.2

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. 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
1	LLP	B	230	24/25	0.97	0.08	6,24,45,52	0
1	LLP	A	230	24/25	0.98	0.08	4,18,25,33	0

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($\text{\AA}^2$)	Q<0.9
2	OOO	A	401	11/11	0.97	0.09	20,31,48,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.