



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 6, 2017 – 03:16 PM EST

PDB ID : 5B1H  
Title : Crystal structure of cystathionine beta-synthase from *Lactobacillus plantarum*  
Authors : Matoba, Y.; Sugiyama, M.  
Deposited on : 2015-12-04  
Resolution : 2.40 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](mailto: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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

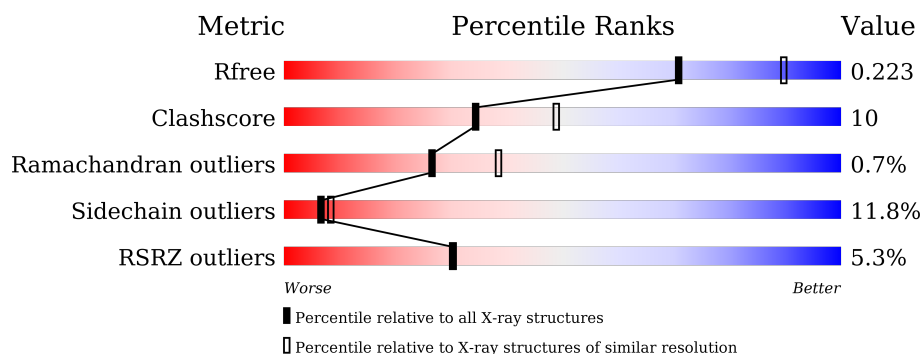
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	311	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>• •</div> </div> </div>
1	B	311	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>• •</div> </div> </div>
1	C	311	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>• •</div> </div> </div>
1	D	311	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>• •</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	406	-	-	-	X
3	GOL	A	407	-	-	-	X
3	GOL	B	403	-	-	-	X
3	GOL	B	405	-	-	-	X
3	GOL	B	406	-	-	-	X
3	GOL	C	405	-	-	-	X
3	GOL	C	406	-	-	-	X
3	GOL	D	404	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9736 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 Cystathionine beta-synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	P	S	0	2	0
			2294	1454	401	431	1	7			
1	B	303	Total	C	N	O	P	S	0	3	0
			2299	1457	403	431	1	7			
1	C	303	Total	C	N	O	P	S	0	2	0
			2294	1454	401	431	1	7			
1	D	303	Total	C	N	O	P	S	0	3	0
			2299	1457	403	431	1	7			

There are 32 discrepancies between the modelled and reference sequences:

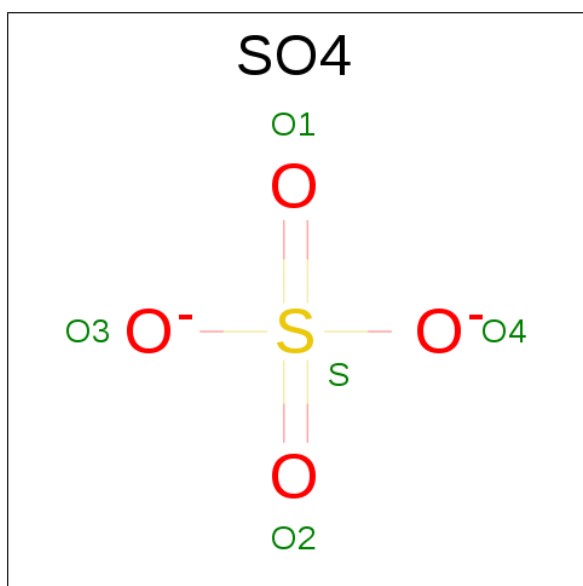
Chain	Residue	Modelled	Actual	Comment	Reference
A	304	LEU	-	expression tag	UNP F9UT54
A	305	GLU	-	expression tag	UNP F9UT54
A	306	HIS	-	expression tag	UNP F9UT54
A	307	HIS	-	expression tag	UNP F9UT54
A	308	HIS	-	expression tag	UNP F9UT54
A	309	HIS	-	expression tag	UNP F9UT54
A	310	HIS	-	expression tag	UNP F9UT54
A	311	HIS	-	expression tag	UNP F9UT54
B	304	LEU	-	expression tag	UNP F9UT54
B	305	GLU	-	expression tag	UNP F9UT54
B	306	HIS	-	expression tag	UNP F9UT54
B	307	HIS	-	expression tag	UNP F9UT54
B	308	HIS	-	expression tag	UNP F9UT54
B	309	HIS	-	expression tag	UNP F9UT54
B	310	HIS	-	expression tag	UNP F9UT54
B	311	HIS	-	expression tag	UNP F9UT54
C	304	LEU	-	expression tag	UNP F9UT54
C	305	GLU	-	expression tag	UNP F9UT54
C	306	HIS	-	expression tag	UNP F9UT54
C	307	HIS	-	expression tag	UNP F9UT54
C	308	HIS	-	expression tag	UNP F9UT54

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	309	HIS	-	expression tag	UNP F9UT54
C	310	HIS	-	expression tag	UNP F9UT54
C	311	HIS	-	expression tag	UNP F9UT54
D	304	LEU	-	expression tag	UNP F9UT54
D	305	GLU	-	expression tag	UNP F9UT54
D	306	HIS	-	expression tag	UNP F9UT54
D	307	HIS	-	expression tag	UNP F9UT54
D	308	HIS	-	expression tag	UNP F9UT54
D	309	HIS	-	expression tag	UNP F9UT54
D	310	HIS	-	expression tag	UNP F9UT54
D	311	HIS	-	expression tag	UNP F9UT54

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



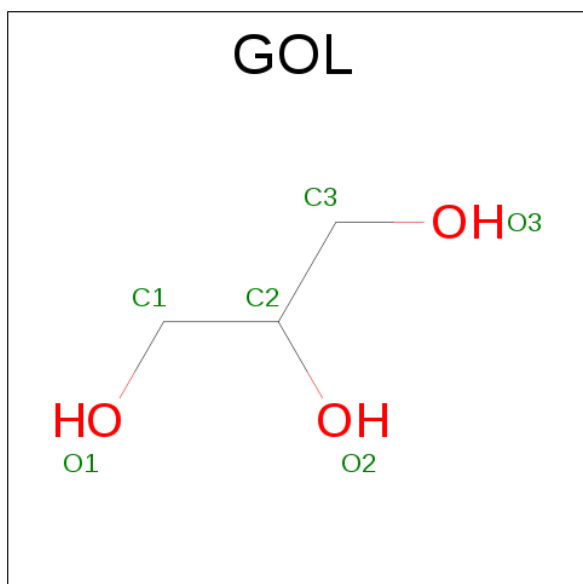
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

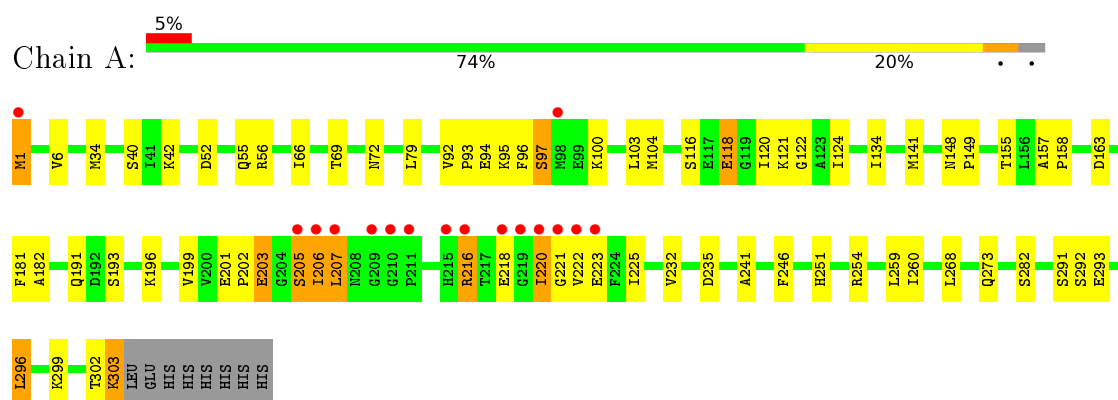
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total	O	0	0
			96	96		
4	B	107	Total	O	0	0
			107	107		
4	C	99	Total	O	0	0
			99	99		
4	D	104	Total	O	0	0
			104	104		

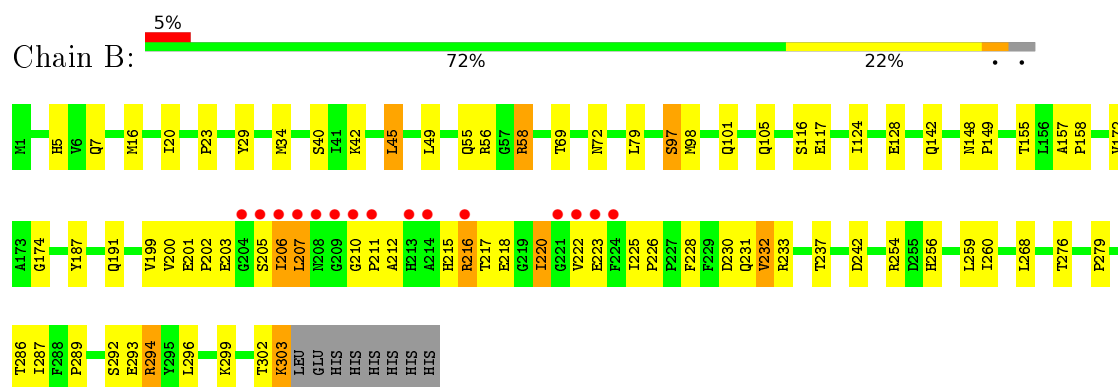
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

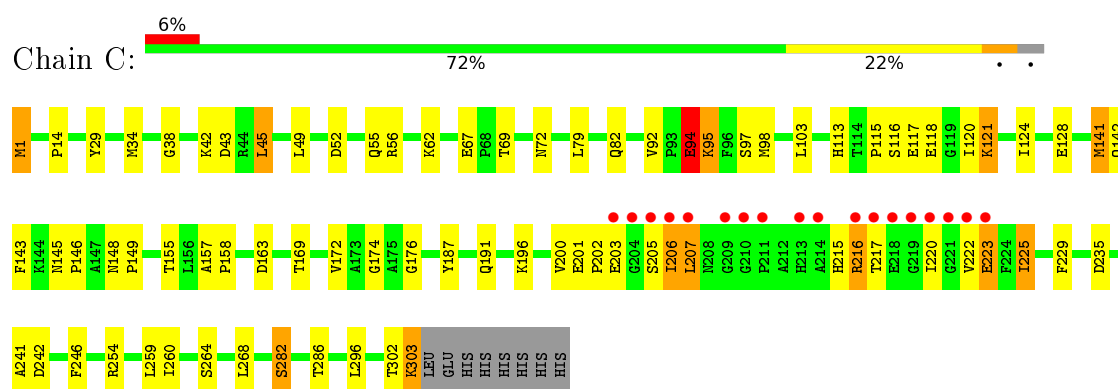
#### • Molecule 1: Cystathionine beta-synthase



#### • Molecule 1: Cystathionine beta-synthase



#### • Molecule 1: Cystathionine beta-synthase





Chain D:

Category	Percentage
M1	5%
H5	74%
V6	74%
Q7	74%
T13	74%
I20	74%
P23	74%
K31	74%
M34	74%
S40	74%
I41	74%
K42	74%
L45	74%
L49	74%
Q55	74%
R56	74%
G57	74%
R58	74%
T69	74%
N72	74%
T73	74%
L77	74%
A78	74%
L79	74%
P83	74%
E94	74%
K95	74%
F96	74%
S97	74%
M98	74%
L103	74%
S116	74%
I124	74%
E128	74%
N148	74%
P149	74%
T155	74%
L156	74%
A157	74%
P159	74%
V172	74%
Y187	74%
Q191	74%
V199	74%
V200	74%
P201	74%
P202	74%
E203	74%
G204	74%
S205	74%
I206	74%
L207	74%
N208	74%
G209	74%
G210	74%
P211	74%
A212	74%
H213	74%
A214	74%
H215	74%
R216	74%
T217	74%
E218	74%
G219	74%
I220	74%
G221	74%
V222	74%
E223	74%
F224	74%
L225	74%
D230	74%
Q231	74%
V232	74%
R233	74%
D242	74%
F246	74%
R254	74%
D255	74%
H256	74%
L259	74%
I260	74%
L268	74%
Q273	74%
T276	74%
T286	74%
S292	74%
E293	74%
R294	74%
Y295	74%
L296	74%
S297	74%
K299	74%
T302	74%
K303	74%
LEU	74%
GLU	74%
HIS	74%
HIS	74%
HIS	74%
HIS	74%
HIS	74%

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.89Å 146.34Å 82.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.49 – 2.40 46.06 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.49-2.40) 97.1 (46.06-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.189 , 0.221 0.190 , 0.223	Depositor DCC
$R_{free}$ test set	3181 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.047 for k,h,-l 0.046 for -k,-h,-l 0.478 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9736	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: GOL, LLP, 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	0/2330	0.57	0/3171
1	B	0.33	0/2341	0.58	0/3186
1	C	0.32	0/2330	0.57	1/3171 (0.0%)
1	D	0.33	0/2341	0.59	0/3186
All	All	0.32	0/9342	0.57	1/12714 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	GLY	N-CA-C	-5.16	100.20	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	2294	0	2295	45	0
1	B	2299	0	2298	43	0
1	C	2294	0	2295	57	0
1	D	2299	0	2298	44	0
2	A	20	0	0	0	0
2	B	10	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	20	0	0	0	0
2	D	10	0	0	0	0
3	A	24	0	32	1	0
3	B	24	0	32	1	0
3	C	18	0	24	0	0
3	D	18	0	24	0	0
4	A	96	0	0	4	0
4	B	107	0	0	1	0
4	C	99	0	0	1	0
4	D	104	0	0	1	0
All	All	9736	0	9298	186	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 10.

The worst 5 of 186 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:1:MET:HG2	1:C:14:PRO:HA	1.43	1.00
1:A:203:GLU:HG2	1:A:241:ALA:HA	1.43	0.98
1:D:201:GLU:OE1	1:D:207:LEU:HB2	1.68	0.94
1:B:202:PRO:HD3	1:B:220:ILE:HD12	1.51	0.92
1:A:1:MET:HA	4:A:577:HOH:O	1.70	0.90

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	302/311 (97%)	290 (96%)	11 (4%)	1 (0%)	46 63
1	B	303/311 (97%)	290 (96%)	9 (3%)	4 (1%)	15 21

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	302/311 (97%)	293 (97%)	7 (2%)	2 (1%)	26	38
1	D	303/311 (97%)	288 (95%)	14 (5%)	1 (0%)	46	63
All	All	1210/1244 (97%)	1161 (96%)	41 (3%)	8 (1%)	26	38

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	97	SER
1	B	211	PRO
1	C	97	SER
1	D	97	SER
1	C	94	GLU

### 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	237/243 (98%)	206 (87%)	31 (13%)	5	6
1	B	238/243 (98%)	210 (88%)	28 (12%)	6	8
1	C	237/243 (98%)	209 (88%)	28 (12%)	6	8
1	D	238/243 (98%)	213 (90%)	25 (10%)	8	12
All	All	950/972 (98%)	838 (88%)	112 (12%)	6	8

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	254[A]	ARG
1	C	55	GLN
1	D	268	LEU
1	B	259	LEU
1	B	296	LEU

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	D	25	HIS
1	D	55	GLN
1	D	208	ASN
1	B	236	GLN
1	D	84	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 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	42	1	22,24,25	2.09	8 (36%)	28,32,34	1.25	4 (14%)
1	LLP	B	42	1	22,24,25	1.95	8 (36%)	28,32,34	1.26	4 (14%)
1	LLP	C	42	1	22,24,25	2.03	8 (36%)	28,32,34	1.23	3 (10%)
1	LLP	D	42	1	22,24,25	1.96	8 (36%)	28,32,34	1.26	3 (10%)

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	42	1	-	0/15/17/19	0/1/1/1
1	LLP	B	42	1	-	0/15/17/19	0/1/1/1
1	LLP	C	42	1	-	0/15/17/19	0/1/1/1
1	LLP	D	42	1	-	0/15/17/19	0/1/1/1

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	LLP	O3-C3	-4.67	1.26	1.37
1	C	42	LLP	O3-C3	-4.67	1.26	1.37
1	D	42	LLP	O3-C3	-4.60	1.26	1.37
1	B	42	LLP	O3-C3	-4.51	1.26	1.37
1	D	42	LLP	OP4-C5'	-2.12	1.36	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	LLP	CE-NZ-C4'	-2.96	110.31	119.14
1	D	42	LLP	C4-C4'-NZ	-2.82	109.43	125.14
1	C	42	LLP	CE-NZ-C4'	-2.80	110.78	119.14
1	B	42	LLP	C4-C4'-NZ	-2.72	110.04	125.14
1	D	42	LLP	CE-NZ-C4'	-2.65	111.24	119.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	42	LLP	3	0
1	B	42	LLP	3	0
1	C	42	LLP	3	0
1	D	42	LLP	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

26 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	SO4	A	401	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	A	402	-	4,4,4	0.21	0	6,6,6	0.08	0
2	SO4	A	403	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	A	404	-	4,4,4	0.20	0	6,6,6	0.05	0
3	GOL	A	405	-	5,5,5	0.28	0	5,5,5	0.18	0
3	GOL	A	406	-	5,5,5	0.31	0	5,5,5	0.24	0
3	GOL	A	407	-	5,5,5	0.20	0	5,5,5	0.23	0
3	GOL	A	408	-	5,5,5	0.24	0	5,5,5	0.21	0
2	SO4	B	401	-	4,4,4	0.21	0	6,6,6	0.09	0
2	SO4	B	402	-	4,4,4	0.23	0	6,6,6	0.11	0
3	GOL	B	403	-	5,5,5	0.28	0	5,5,5	0.20	0
3	GOL	B	404	-	5,5,5	0.30	0	5,5,5	0.24	0
3	GOL	B	405	-	5,5,5	0.29	0	5,5,5	0.20	0
3	GOL	B	406	-	5,5,5	0.29	0	5,5,5	0.23	0
2	SO4	C	401	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	C	402	-	4,4,4	0.20	0	6,6,6	0.13	0
2	SO4	C	403	-	4,4,4	0.25	0	6,6,6	0.17	0
2	SO4	C	404	-	4,4,4	0.22	0	6,6,6	0.09	0
3	GOL	C	405	-	5,5,5	0.37	0	5,5,5	0.22	0
3	GOL	C	406	-	5,5,5	0.24	0	5,5,5	0.25	0
3	GOL	C	407	-	5,5,5	0.33	0	5,5,5	0.24	0
2	SO4	D	401	-	4,4,4	0.18	0	6,6,6	0.09	0
2	SO4	D	402	-	4,4,4	0.18	0	6,6,6	0.09	0
3	GOL	D	403	-	5,5,5	0.33	0	5,5,5	0.24	0
3	GOL	D	404	-	5,5,5	0.21	0	5,5,5	0.19	0
3	GOL	D	405	-	5,5,5	0.32	0	5,5,5	0.25	0

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	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	A	402	-	-	0/0/0/0	0/0/0/0
2	SO4	A	403	-	-	0/0/0/0	0/0/0/0
2	SO4	A	404	-	-	0/0/0/0	0/0/0/0
3	GOL	A	405	-	-	0/4/4/4	0/0/0/0
3	GOL	A	406	-	-	0/4/4/4	0/0/0/0
3	GOL	A	407	-	-	0/4/4/4	0/0/0/0
3	GOL	A	408	-	-	0/4/4/4	0/0/0/0
2	SO4	B	401	-	-	0/0/0/0	0/0/0/0
2	SO4	B	402	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	B	404	-	-	0/4/4/4	0/0/0/0
3	GOL	B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	B	406	-	-	0/4/4/4	0/0/0/0
2	SO4	C	401	-	-	0/0/0/0	0/0/0/0
2	SO4	C	402	-	-	0/0/0/0	0/0/0/0
2	SO4	C	403	-	-	0/0/0/0	0/0/0/0
2	SO4	C	404	-	-	0/0/0/0	0/0/0/0
3	GOL	C	405	-	-	0/4/4/4	0/0/0/0
3	GOL	C	406	-	-	0/4/4/4	0/0/0/0
3	GOL	C	407	-	-	0/4/4/4	0/0/0/0
2	SO4	D	401	-	-	0/0/0/0	0/0/0/0
2	SO4	D	402	-	-	0/0/0/0	0/0/0/0
3	GOL	D	403	-	-	0/4/4/4	0/0/0/0
3	GOL	D	404	-	-	0/4/4/4	0/0/0/0
3	GOL	D	405	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	406	GOL	1	0
3	B	406	GOL	1	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, 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	302/311 (97%)	-0.13	16 (5%) 30 30	32, 45, 102, 117	0
1	B	302/311 (97%)	-0.07	15 (4%) 32 33	33, 44, 106, 126	0
1	C	302/311 (97%)	-0.13	18 (5%) 25 25	33, 46, 101, 120	0
1	D	302/311 (97%)	-0.11	15 (4%) 32 33	33, 44, 107, 125	0
All	All	1208/1244 (97%)	-0.11	64 (5%) 30 30	32, 45, 105, 126	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	ALA	8.6
1	B	211	PRO	7.4
1	B	222	VAL	7.2
1	A	206	ILE	6.7
1	B	210	GLY	6.7

### 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	LLP	B	42	24/25	0.98	0.12	-	36,40,44,45	0
1	LLP	D	42	24/25	0.98	0.12	-	35,39,42,44	0
1	LLP	A	42	24/25	0.98	0.12	-	38,46,48,48	0
1	LLP	C	42	24/25	0.97	0.14	-	37,45,47,48	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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	C	405	6/6	0.91	0.26	12.53	73,74,75,76	0
3	GOL	B	406	6/6	0.94	0.20	10.67	68,70,70,71	0
3	GOL	B	405	6/6	0.88	0.29	8.23	80,81,82,82	0
3	GOL	B	403	6/6	0.87	0.24	7.67	76,83,83,84	0
3	GOL	A	406	6/6	0.86	0.30	6.90	59,63,63,65	0
3	GOL	C	406	6/6	0.90	0.25	6.19	72,74,74,74	0
3	GOL	D	404	6/6	0.80	0.36	5.64	89,91,92,92	0
3	GOL	A	407	6/6	0.94	0.19	3.40	71,72,73,74	0
3	GOL	D	403	6/6	0.86	0.14	1.79	66,74,75,75	0
2	SO4	D	401	5/5	0.86	0.20	1.38	125,126,126,127	0
2	SO4	B	402	5/5	0.88	0.17	1.25	111,113,113,114	0
2	SO4	C	402	5/5	0.79	0.21	1.21	124,125,125,126	0
3	GOL	A	405	6/6	0.71	0.20	0.85	95,95,96,96	0
3	GOL	C	407	6/6	0.90	0.14	0.29	72,75,76,77	0
2	SO4	A	404	5/5	0.90	0.15	0.04	116,117,117,118	0
2	SO4	B	401	5/5	0.98	0.10	-	78,80,81,82	0
2	SO4	C	401	5/5	0.93	0.10	-	91,91,92,92	0
2	SO4	C	403	5/5	0.95	0.25	-	76,79,81,81	0
2	SO4	A	402	5/5	0.87	0.28	-	97,99,100,101	0
2	SO4	C	404	5/5	0.92	0.29	-	98,100,101,102	0
3	GOL	D	405	6/6	0.93	0.19	-	74,76,77,77	0
2	SO4	D	402	5/5	0.98	0.08	-	79,80,81,82	0
3	GOL	A	408	6/6	0.89	0.18	-	71,76,76,77	0
3	GOL	B	404	6/6	0.93	0.11	-	82,85,86,86	0
2	SO4	A	403	5/5	0.90	0.28	-	80,82,85,85	0
2	SO4	A	401	5/5	0.94	0.14	-	93,93,94,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.