



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:36 am BST

PDB ID : 3QHX  
Title : Crystal Structure of Cystathionine gamma-synthase MetB (Cgs) from Mycobacterium ulcerans Agy99 bound to HEPES  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2011-01-26  
Resolution : 1.65 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

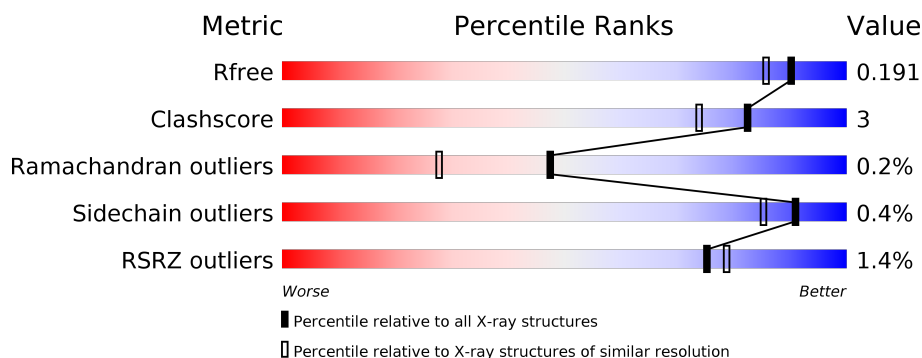
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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))
$R_{free}$	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 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	392	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>86%</span> <span>10%</span> <span>• •</span> </div> </div>
1	B	392	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>84%</span> <span>10%</span> <span>6%</span> </div> </div>
1	C	392	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>85%</span> <span>8%</span> <span>6%</span> </div> </div>
1	D	392	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>85%</span> <span>11%</span> <span>•</span> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12719 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 gamma-synthase MetB (Cgs).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	P	S	0	14	0
			2844	1790	494	548	1	11			
1	B	370	Total	C	N	O	P	S	0	13	0
			2781	1755	476	539	1	10			
1	C	369	Total	C	N	O	P	S	0	11	0
			2759	1737	479	532	1	10			
1	D	377	Total	C	N	O	P	S	0	10	0
			2796	1761	485	538	1	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP A0PKT3
A	-2	PRO	-	EXPRESSION TAG	UNP A0PKT3
A	-1	GLY	-	EXPRESSION TAG	UNP A0PKT3
A	0	SER	-	EXPRESSION TAG	UNP A0PKT3
B	-3	GLY	-	EXPRESSION TAG	UNP A0PKT3
B	-2	PRO	-	EXPRESSION TAG	UNP A0PKT3
B	-1	GLY	-	EXPRESSION TAG	UNP A0PKT3
B	0	SER	-	EXPRESSION TAG	UNP A0PKT3
C	-3	GLY	-	EXPRESSION TAG	UNP A0PKT3
C	-2	PRO	-	EXPRESSION TAG	UNP A0PKT3
C	-1	GLY	-	EXPRESSION TAG	UNP A0PKT3
C	0	SER	-	EXPRESSION TAG	UNP A0PKT3
D	-3	GLY	-	EXPRESSION TAG	UNP A0PKT3
D	-2	PRO	-	EXPRESSION TAG	UNP A0PKT3
D	-1	GLY	-	EXPRESSION TAG	UNP A0PKT3
D	0	SER	-	EXPRESSION TAG	UNP A0PKT3

- 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	B	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		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total 1	Na 1	0	0

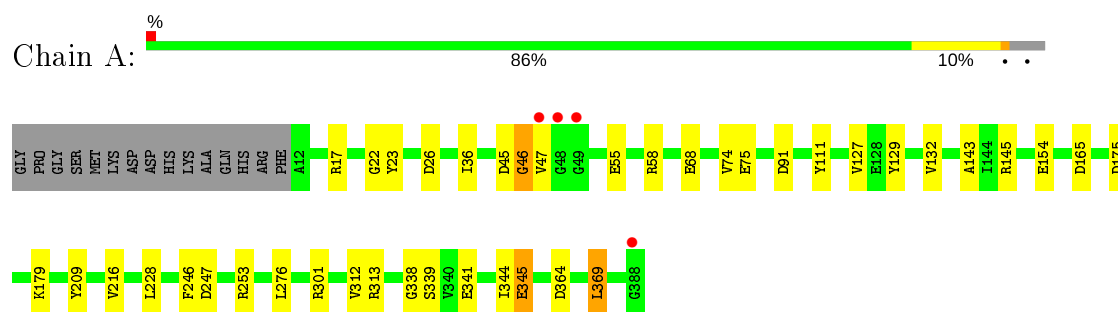
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	408	Total 408	O 408	0	0
6	B	360	Total 360	O 360	0	0
6	C	354	Total 354	O 354	0	0
6	D	365	Total 365	O 365	0	0

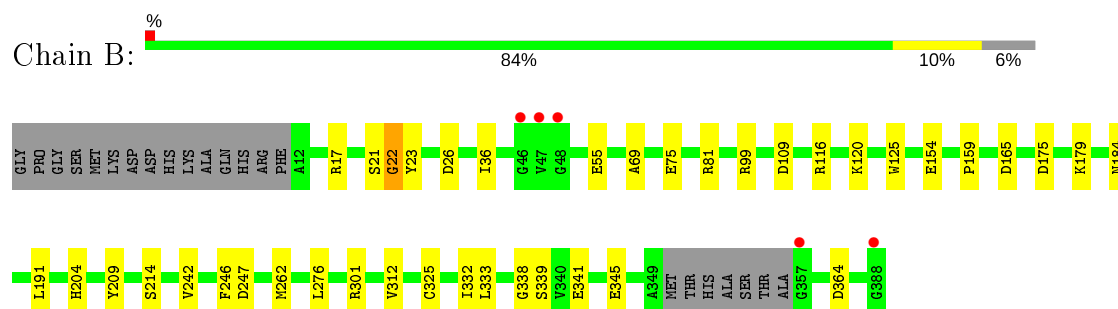
### 3 Residue-property plots [i](#)

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.

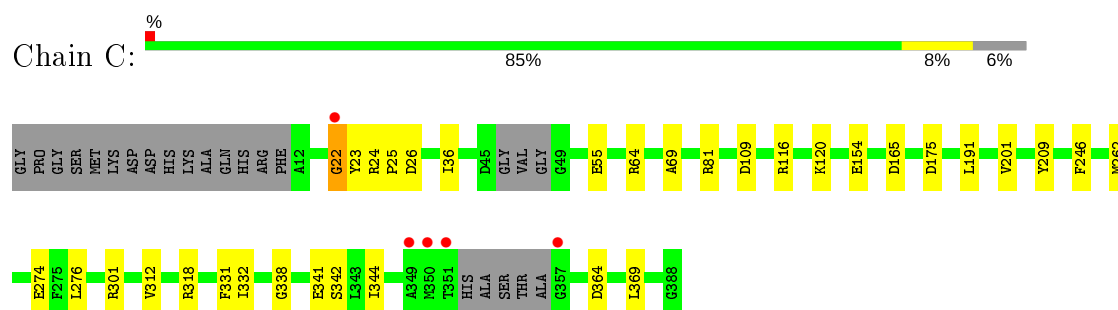
- Molecule 1: Cystathionine gamma-synthase MetB (Cgs)



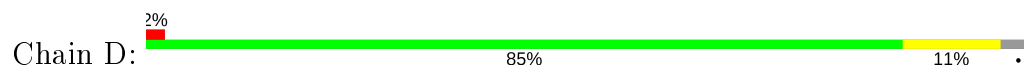
- Molecule 1: Cystathionine gamma-synthase MetB (Cgs)

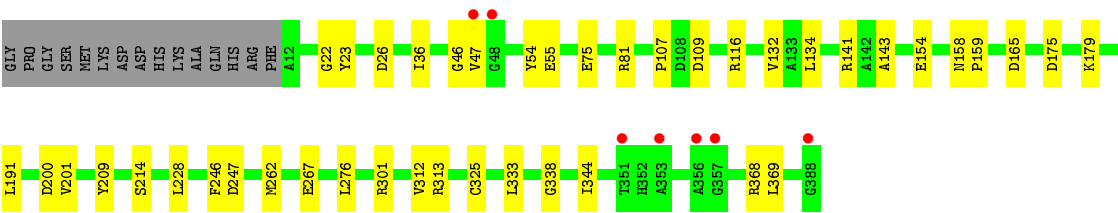


- Molecule 1: Cystathionine gamma-synthase MetB (Cgs)



- Molecule 1: Cystathionine gamma-synthase MetB (Cgs)







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.96Å 106.33Å 100.55Å 90.00° 113.72° 90.00°	Depositor
Resolution (Å)	29.23 – 1.65 29.23 – 1.65	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.23-1.65) 97.7 (29.23-1.65)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.72 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.148 , 0.181 0.163 , 0.191	Depositor DCC
$R_{free}$ test set	9180 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.7	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.57$ , $\langle L^2 \rangle = 0.42$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12719	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4798e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: EPE, GOL, LLP, SO4, NA

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	1.29	13/2910 (0.4%)	1.15	20/3965 (0.5%)
1	B	1.32	15/2842 (0.5%)	1.12	17/3874 (0.4%)
1	C	1.26	10/2815 (0.4%)	1.12	14/3836 (0.4%)
1	D	1.36	16/2852 (0.6%)	1.12	17/3891 (0.4%)
All	All	1.31	54/11419 (0.5%)	1.13	68/15566 (0.4%)

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
1	A	0	1
1	D	0	1
All	All	0	2

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	23	TYR	CD2-CE2	-13.12	1.19	1.39
1	D	154	GLU	CD-OE1	12.39	1.39	1.25
1	D	154	GLU	CB-CG	-11.93	1.29	1.52
1	B	23	TYR	CD2-CE2	-9.56	1.25	1.39
1	B	55	GLU	CB-CG	-8.97	1.35	1.52
1	D	26	ASP	CB-CG	-8.72	1.33	1.51
1	D	179	LYS	CD-CE	8.26	1.71	1.51
1	D	154	GLU	CG-CD	8.04	1.64	1.51
1	D	75	GLU	CG-CD	7.93	1.63	1.51
1	A	26	ASP	CB-CG	-7.85	1.35	1.51
1	B	154	GLU	CG-CD	7.68	1.63	1.51
1	D	154	GLU	CD-OE2	-7.60	1.17	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	55	GLU	CB-CG	-7.58	1.37	1.52
1	C	26	ASP	CB-CG	-7.43	1.36	1.51
1	B	55	GLU	CG-CD	7.21	1.62	1.51
1	A	75	GLU	CG-CD	6.89	1.62	1.51
1	C	120	LYS	CE-NZ	6.85	1.66	1.49
1	C	154	GLU	CG-CD	6.85	1.62	1.51
1	D	55	GLU	CG-CD	6.70	1.62	1.51
1	A	23	TYR	CD2-CE2	-6.60	1.29	1.39
1	B	120	LYS	CE-NZ	6.38	1.65	1.49
1	C	23	TYR	CD2-CE2	-6.26	1.29	1.39
1	B	154	GLU	CB-CG	-6.26	1.40	1.52
1	B	247	ASP	CB-CG	6.22	1.64	1.51
1	B	116	ARG	CZ-NH1	6.09	1.41	1.33
1	B	26	ASP	CB-CG	-6.07	1.39	1.51
1	A	179	LYS	CD-CE	6.04	1.66	1.51
1	A	111	TYR	CE2-CZ	-6.03	1.30	1.38
1	C	55	GLU	CG-CD	6.02	1.60	1.51
1	B	179	LYS	CD-CE	6.01	1.66	1.51
1	B	214	SER	CB-OG	-6.01	1.34	1.42
1	A	301	ARG	CB-CG	-5.99	1.36	1.52
1	A	127	VAL	CB-CG1	5.93	1.65	1.52
1	D	267	GLU	CD-OE2	5.92	1.32	1.25
1	A	154	GLU	CG-CD	5.86	1.60	1.51
1	B	75	GLU	CG-CD	5.79	1.60	1.51
1	B	345	GLU	CB-CG	-5.76	1.41	1.52
1	C	55	GLU	CB-CG	-5.73	1.41	1.52
1	A	55	GLU	CG-CD	5.69	1.60	1.51
1	D	54	TYR	CD2-CE2	5.68	1.47	1.39
1	C	201	VAL	CB-CG1	-5.67	1.41	1.52
1	A	74	VAL	CB-CG1	5.64	1.64	1.52
1	D	214	SER	CB-OG	-5.42	1.35	1.42
1	B	301	ARG	CB-CG	-5.35	1.38	1.52
1	D	158	ASN	CG-ND2	5.33	1.46	1.32
1	A	345	GLU	CD-OE1	5.32	1.31	1.25
1	B	23	TYR	CB-CG	-5.26	1.43	1.51
1	A	216	VAL	CB-CG1	5.26	1.63	1.52
1	D	116	ARG	CG-CD	5.24	1.65	1.51
1	A	68	GLU	CD-OE1	5.17	1.31	1.25
1	C	301	ARG	CB-CG	-5.16	1.38	1.52
1	C	341	GLU	CB-CG	-5.08	1.42	1.52
1	C	154	GLU	CB-CG	-5.06	1.42	1.52
1	D	54	TYR	CE2-CZ	-5.05	1.31	1.38

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	C	318	ARG	NE-CZ-NH2	9.02	124.81	120.30
1	C	318	ARG	NE-CZ-NH1	-8.01	116.30	120.30
1	D	154	GLU	CG-CD-OE2	-7.91	102.48	118.30
1	C	301	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	B	26	ASP	CB-CG-OD1	-7.82	111.26	118.30
1	A	17	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	D	247	ASP	CB-CG-OD2	-7.56	111.49	118.30
1	A	154	GLU	OE1-CD-OE2	7.48	132.28	123.30
1	B	81	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	A	165	ASP	CB-CG-OD1	7.39	124.95	118.30
1	A	301	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	B	165	ASP	CB-CG-OD1	6.99	124.59	118.30
1	D	301	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	A	17	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	22[A]	GLY	N-CA-C	-6.62	96.54	113.10
1	B	22[B]	GLY	N-CA-C	-6.62	96.54	113.10
1	B	21	SER	O-C-N	-6.62	111.94	123.20
1	D	23	TYR	CD1-CE1-CZ	-6.51	113.94	119.80
1	A	301	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	D	23	TYR	CB-CG-CD2	-6.50	117.10	121.00
1	C	26	ASP	N-CA-CB	-6.47	98.96	110.60
1	A	26	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	D	154	GLU	OE1-CD-OE2	6.32	130.88	123.30
1	B	154	GLU	OE1-CD-OE2	6.28	130.84	123.30
1	C	301	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	D	175	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	A	364	ASP	CB-CG-OD2	6.07	123.77	118.30
1	B	99	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	D	368	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	D	81	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	A	253	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	D	109	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	228	LEU	CB-CG-CD1	-5.88	101.00	111.00
1	C	64	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	D	26	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	A	165	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	B	116	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	109	ASP	CB-CG-OD1	5.74	123.47	118.30
1	C	26	ASP	CB-CG-OD1	-5.73	113.14	118.30
1	D	313	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	C	364	ASP	CB-CG-OD1	-5.64	113.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	165	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	145	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	200	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	A	175	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	C	165	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	17	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	47	VAL	CB-CA-C	5.43	121.71	111.40
1	A	247	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	21	SER	C-N-CA	-5.37	111.02	122.30
1	D	75	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	A	313	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	C	109	ASP	CB-CG-OD1	5.29	123.07	118.30
1	A	17	ARG	CG-CD-NE	-5.28	100.72	111.80
1	B	247	ASP	CB-CG-OD1	5.26	123.04	118.30
1	C	81	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	91	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	D	247	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	129	TYR	CB-CG-CD1	5.15	124.09	121.00
1	B	175	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	B	364	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	B	242	VAL	CG1-CB-CG2	5.11	119.08	110.90
1	C	175	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	58	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	D	23	TYR	OH-CZ-CE2	-5.05	106.46	120.10
1	C	22[A]	GLY	N-CA-C	-5.03	100.53	113.10
1	C	22[B]	GLY	N-CA-C	-5.03	100.53	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22[B]	GLY	Peptide
1	D	22[A]	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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	2844	0	2820	16	0
1	B	2781	0	2747	18	0
1	C	2759	0	2722	15	0
1	D	2796	0	2759	13	0
2	A	5	0	0	0	0
2	B	15	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	15	0	17	0	0
4	A	6	0	8	1	0
5	C	1	0	0	0	0
6	A	408	0	0	0	0
6	B	360	0	0	0	0
6	C	354	0	0	3	0
6	D	365	0	0	1	0
All	All	12719	0	11073	56	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 3.

All (56) 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:B:332[A]:ILE:HD11	1:B:341[A]:GLU:OE2	1.59	1.02
1:B:332[A]:ILE:CD1	1:B:341[A]:GLU:CD	2.52	0.78
1:B:332[A]:ILE:CD1	1:B:341[A]:GLU:OE2	2.34	0.74
1:C:274[B]:GLU:OE1	6:C:2370:HOH:O	2.07	0.73
1:B:332[A]:ILE:HD12	1:B:341[A]:GLU:CD	2.09	0.72
1:B:339:SER:OG	1:B:341[B]:GLU:OE1	2.10	0.68
1:B:332[A]:ILE:HD11	1:B:341[A]:GLU:CD	2.15	0.67
1:A:45:ASP:O	1:A:46:GLY:O	2.22	0.57
1:C:332:ILE:HD12	6:C:1382:HOH:O	2.05	0.57
1:A:45:ASP:C	1:A:46:GLY:O	2.45	0.54
4:A:391:GOL:H12	1:B:125:TRP:CE2	2.42	0.54
1:A:344:ILE:HG13	1:A:369[B]:LEU:HD23	1.90	0.52
1:B:22[A]:GLY:HA2	1:B:69:ALA:CB	2.40	0.52
1:A:344:ILE:HD12	1:A:369[B]:LEU:CD2	2.40	0.51
1:A:344:ILE:HD12	1:A:369[B]:LEU:HD21	1.93	0.51
1:B:276:LEU:HD13	1:B:312:VAL:HG11	1.93	0.50
1:B:184:ASN:HB3	1:B:204:HIS:CE1	2.46	0.50
1:A:344:ILE:CD1	1:A:369[B]:LEU:HD21	2.43	0.49
1:B:22[A]:GLY:HA2	1:B:69:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ILE:HB	1:D:36:ILE:HB	1.93	0.49
1:D:276:LEU:HD13	1:D:312:VAL:HG11	1.95	0.48
1:A:246[A]:PHE:HE1	1:D:246:PHE:CD1	2.31	0.48
1:C:276:LEU:HD13	1:C:312:VAL:HG11	1.96	0.48
1:B:22[B]:GLY:HA2	1:B:69:ALA:HB1	1.96	0.47
1:D:201[A]:VAL:HG22	1:D:228:LEU:HD13	1.97	0.47
1:A:276:LEU:HD13	1:A:312:VAL:HG11	1.96	0.47
1:B:36:ILE:HB	1:C:36:ILE:HB	1.95	0.47
1:D:209:TYR:CE1	1:D:338:GLY:HA2	2.49	0.47
1:B:22[B]:GLY:HA2	1:B:69:ALA:CB	2.44	0.47
1:B:325:CYS:HB3	1:B:333:LEU:HD13	1.95	0.47
1:B:191:LEU:HG	1:B:262[B]:MET:HG2	1.97	0.46
1:C:209:TYR:CE1	1:C:338:GLY:HA2	2.51	0.46
1:D:325:CYS:HB3	1:D:333:LEU:HD13	1.99	0.45
1:C:344:ILE:HG13	1:C:369[A]:LEU:HD13	1.99	0.45
1:A:132[B]:VAL:HG21	1:A:143:ALA:CB	2.47	0.44
1:C:22[B]:GLY:HA2	1:C:69:ALA:HB1	1.99	0.44
1:D:132[B]:VAL:HG21	1:D:143:ALA:HB2	2.00	0.44
1:C:116[B]:ARG:NH2	6:C:774:HOH:O	2.42	0.43
1:C:22[A]:GLY:HA2	1:C:69:ALA:HB1	2.00	0.43
1:C:22[A]:GLY:HA2	1:C:69:ALA:CB	2.48	0.43
1:D:141[B]:ARG:NH2	6:D:850:HOH:O	2.51	0.43
1:A:246[A]:PHE:CD1	1:D:246:PHE:HE1	2.37	0.42
1:A:246[A]:PHE:HE1	1:D:246:PHE:HD1	1.67	0.42
1:D:107:PRO:HG3	1:D:134:LEU:HD11	2.02	0.42
1:D:344:ILE:HD12	1:D:369[A]:LEU:CD2	2.50	0.42
1:A:209:TYR:CE1	1:A:338:GLY:HA2	2.55	0.42
1:A:339:SER:OG	1:A:341[A]:GLU:OE1	2.34	0.41
1:B:246[A]:PHE:HE1	1:C:246:PHE:CD1	2.38	0.41
1:D:191:LEU:HG	1:D:262[B]:MET:HG2	2.02	0.41
1:B:209:TYR:CE1	1:B:338:GLY:HA2	2.56	0.41
1:C:331:PHE:CD1	1:C:342:SER:HB3	2.55	0.41
1:A:132[B]:VAL:HG21	1:A:143:ALA:HB2	2.02	0.41
1:C:24:ARG:O	1:C:25:PRO:C	2.58	0.41
1:C:209:TYR:CD1	1:C:262[A]:MET:SD	3.14	0.41
1:C:191:LEU:HG	1:C:262[B]:MET:HG2	2.03	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	388/392 (99%)	379 (98%)	8 (2%)	1 (0%)	41	22
1	B	378/392 (96%)	372 (98%)	6 (2%)	0	100	100
1	C	373/392 (95%)	369 (99%)	4 (1%)	0	100	100
1	D	384/392 (98%)	372 (97%)	10 (3%)	2 (0%)	29	11
All	All	1523/1568 (97%)	1492 (98%)	28 (2%)	3 (0%)	47	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	47	VAL
1	A	46	GLY
1	D	46	GLY

### 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	290/292 (99%)	287 (99%)	3 (1%)	76	62
1	B	283/292 (97%)	282 (100%)	1 (0%)	91	85
1	C	279/292 (96%)	279 (100%)	0	100	100
1	D	281/292 (96%)	280 (100%)	1 (0%)	91	85
All	All	1133/1168 (97%)	1128 (100%)	5 (0%)	91	85

All (5) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	345	GLU
1	A	369[A]	LEU
1	A	369[B]	LEU
1	B	159	PRO
1	D	159	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	B	208	1	23,24,25	1.83	8 (34%)	25,32,34	1.95	7 (28%)
1	LLP	C	208	1	23,24,25	1.93	8 (34%)	25,32,34	1.60	6 (24%)
1	LLP	A	208	1	23,24,25	1.86	7 (30%)	25,32,34	1.71	6 (24%)
1	LLP	D	208	1	23,24,25	1.87	6 (26%)	25,32,34	2.06	8 (32%)

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	B	208	1	-	4/16/17/19	0/1/1/1
1	LLP	C	208	1	-	3/16/17/19	0/1/1/1
1	LLP	A	208	1	-	3/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	D	208	1	-	4/16/17/19	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	LLP	C4'-NZ	4.07	1.40	1.27
1	D	208	LLP	CD-CE	3.96	1.65	1.51
1	B	208	LLP	C4'-NZ	3.92	1.40	1.27
1	A	208	LLP	O3-C3	-3.84	1.28	1.37
1	C	208	LLP	O3-C3	-3.82	1.28	1.37
1	D	208	LLP	O3-C3	-3.78	1.28	1.37
1	C	208	LLP	C4'-NZ	3.78	1.39	1.27
1	D	208	LLP	CB-CA	3.57	1.58	1.53
1	B	208	LLP	O3-C3	-3.39	1.29	1.37
1	B	208	LLP	CD-CE	3.31	1.63	1.51
1	C	208	LLP	CD-CE	3.27	1.62	1.51
1	A	208	LLP	C4-C4'	3.11	1.52	1.46
1	A	208	LLP	C2'-C2	2.91	1.55	1.50
1	B	208	LLP	C6-N1	2.72	1.40	1.34
1	C	208	LLP	C4-C4'	2.70	1.51	1.46
1	D	208	LLP	C4'-NZ	2.68	1.36	1.27
1	D	208	LLP	C6-N1	2.43	1.39	1.34
1	C	208	LLP	C3-C2	-2.41	1.38	1.40
1	D	208	LLP	CE-NZ	2.40	1.52	1.46
1	C	208	LLP	C6-N1	2.30	1.39	1.34
1	B	208	LLP	C2-N1	2.28	1.38	1.33
1	C	208	LLP	CB-CA	2.28	1.56	1.53
1	C	208	LLP	C4-C3	2.21	1.44	1.40
1	A	208	LLP	CD-CE	2.20	1.59	1.51
1	A	208	LLP	C4-C3	2.14	1.44	1.40
1	B	208	LLP	CD-CG	-2.12	1.39	1.51
1	A	208	LLP	CB-CA	2.11	1.56	1.53
1	B	208	LLP	C4-C4'	2.10	1.50	1.46
1	B	208	LLP	P-OP4	2.10	1.67	1.60

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	LLP	CD-CE-NZ	6.20	126.13	110.93
1	D	208	LLP	C4-C3-C2	-5.17	116.99	120.19
1	D	208	LLP	CD-CE-NZ	4.77	122.63	110.93
1	A	208	LLP	OP2-P-OP4	-3.99	96.11	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	LLP	CD-CE-NZ	3.77	120.16	110.93
1	C	208	LLP	OP2-P-OP4	-3.39	97.72	106.73
1	B	208	LLP	OP2-P-OP4	-3.07	98.56	106.73
1	C	208	LLP	CD-CE-NZ	3.07	118.45	110.93
1	C	208	LLP	C4-C4'-NZ	-2.77	111.61	124.31
1	D	208	LLP	C3-C4-C5	2.74	120.36	118.26
1	B	208	LLP	C5-C6-N1	-2.68	119.36	123.82
1	A	208	LLP	OP4-C5'-C5	2.67	114.45	109.35
1	A	208	LLP	C4-C4'-NZ	-2.61	112.34	124.31
1	D	208	LLP	C5-C6-N1	-2.57	119.53	123.82
1	D	208	LLP	OP4-C5'-C5	2.55	114.22	109.35
1	B	208	LLP	OP2-P-OP1	2.53	120.58	110.68
1	D	208	LLP	OP3-P-OP2	2.50	117.19	107.64
1	D	208	LLP	OP2-P-OP4	-2.47	100.15	106.73
1	C	208	LLP	OP2-P-OP1	2.46	120.30	110.68
1	A	208	LLP	C5'-C5-C6	-2.32	115.55	119.37
1	D	208	LLP	OP2-P-OP1	2.31	119.71	110.68
1	B	208	LLP	C4-C3-C2	-2.31	118.76	120.19
1	C	208	LLP	C5-C4-C4'	-2.23	117.88	121.56
1	B	208	LLP	OP4-C5'-C5	2.14	113.44	109.35
1	B	208	LLP	C4-C4'-NZ	-2.14	114.50	124.31
1	A	208	LLP	OP2-P-OP1	2.12	118.97	110.68
1	C	208	LLP	C2'-C2-C3	2.02	123.38	120.89

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	208	LLP	O-C-CA-CB
1	C	208	LLP	O-C-CA-CB
1	A	208	LLP	O-C-CA-CB
1	D	208	LLP	O-C-CA-CB
1	B	208	LLP	C4-C4'-NZ-CE
1	D	208	LLP	C4-C4'-NZ-CE
1	C	208	LLP	C4-C4'-NZ-CE
1	A	208	LLP	C4-C4'-NZ-CE
1	D	208	LLP	CG-CD-CE-NZ
1	B	208	LLP	CG-CD-CE-NZ
1	B	208	LLP	CA-CB-CG-CD
1	D	208	LLP	CA-CB-CG-CD
1	C	208	LLP	CG-CD-CE-NZ
1	A	208	LLP	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z  > 2$
2	SO4	B	390	-	4,4,4	0.67	0	6,6,6	1.38	1 (16%)
2	SO4	A	389	-	4,4,4	0.49	0	6,6,6	1.45	1 (16%)
2	SO4	C	389	-	4,4,4	0.81	0	6,6,6	0.66	0
3	EPE	A	390	-	15,15,15	1.41	4 (26%)	18,20,20	1.45	3 (16%)
2	SO4	D	389	-	4,4,4	0.73	0	6,6,6	0.98	0
4	GOL	A	391	-	5,5,5	0.77	0	5,5,5	1.12	0
2	SO4	B	389	-	4,4,4	0.27	0	6,6,6	0.81	0
2	SO4	B	391	-	4,4,4	0.39	0	6,6,6	0.95	1 (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
3	EPE	A	390	-	-	0/9/19/19	0/1/1/1
4	GOL	A	391	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	390	EPE	C9-N1	2.68	1.53	1.47
3	A	390	EPE	O1S-S	2.35	1.52	1.45
3	A	390	EPE	C6-N1	2.18	1.52	1.46
3	A	390	EPE	C9-C10	-2.01	1.47	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	390	EPE	C9-N1-C6	3.70	120.70	111.23
3	A	390	EPE	O2S-S-C10	-3.24	103.01	106.92
2	B	390	SO4	O3-S-O1	-2.81	94.62	109.31
2	A	389	SO4	O4-S-O1	-2.69	95.29	109.31
3	A	390	EPE	O8-C8-C7	-2.42	101.13	111.19
2	B	391	SO4	O4-S-O3	2.14	118.21	109.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	391	GOL	C1-C2-C3-O3
4	A	391	GOL	O2-C2-C3-O3
4	A	391	GOL	O1-C1-C2-O2
4	A	391	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	391	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 ⓘ

### 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	376/392 (95%)	-0.44	4 (1%) 80 83	5, 10, 20, 37	1 (0%)
1	B	369/392 (94%)	-0.48	5 (1%) 75 79	5, 10, 21, 35	0
1	C	368/392 (93%)	-0.51	5 (1%) 75 79	5, 10, 20, 40	0
1	D	376/392 (95%)	-0.42	7 (1%) 66 69	5, 10, 22, 39	0
All	All	1489/1568 (94%)	-0.46	21 (1%) 75 79	5, 10, 21, 40	1 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	VAL	6.7
1	A	48	GLY	6.3
1	D	48	GLY	5.3
1	D	47	VAL	4.8
1	D	356	ALA	4.2
1	C	351	THR	4.1
1	A	388	GLY	3.6
1	D	353	ALA	3.5
1	C	357	GLY	3.0
1	D	388	GLY	2.9
1	B	388	GLY	2.8
1	B	48	GLY	2.7
1	C	350	MET	2.6
1	C	22[A]	GLY	2.4
1	D	351	THR	2.4
1	B	357	GLY	2.3
1	D	357	GLY	2.3
1	A	49	GLY	2.3
1	B	46	GLY	2.3
1	B	47	VAL	2.1
1	C	349	ALA	2.1

## 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, 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(Å <sup>2</sup> )	Q<0.9
1	LLP	B	208	24/25	0.98	0.06	4,8,12,16	0
1	LLP	C	208	24/25	0.98	0.07	5,8,15,16	0
1	LLP	D	208	24/25	0.98	0.06	4,8,13,17	0
1	LLP	A	208	24/25	0.99	0.06	4,7,15,16	0

## 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(Å <sup>2</sup> )	Q<0.9
4	GOL	A	391	6/6	0.90	0.12	25,27,28,29	0
2	SO4	A	389	5/5	0.94	0.16	31,31,34,35	0
2	SO4	B	391	5/5	0.94	0.22	39,41,43,46	0
3	EPE	A	390	15/15	0.97	0.09	11,14,19,34	0
2	SO4	D	389	5/5	0.97	0.07	19,21,28,33	0
5	NA	C	390	1/1	0.97	0.09	26,26,26,26	0
2	SO4	B	389	5/5	0.98	0.07	3,6,13,13	5
2	SO4	C	389	5/5	0.98	0.07	24,24,28,36	0
2	SO4	B	390	5/5	0.98	0.11	11,13,18,23	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.