



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 05:40 am BST

PDB ID : 6H2A
Title : Structure of S70A BlaC from Mycobacterium tuberculosis obtained from crystals produced in the presence of DTT
Authors : Tassoni, R.; Pannu, N.S.; Ubbink, M.
Deposited on : 2018-07-13
Resolution : 2.54 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (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

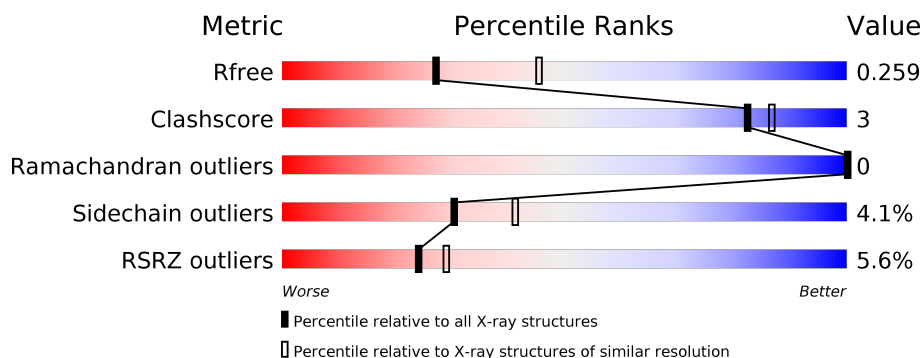
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	274	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 89%, yellow 89%, yellow 96%, grey 96%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 89% 7% • • </div> </div>
1	B	274	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 7%, green 7%, green 91%, yellow 91%, yellow 98%, grey 98%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 7% 91% 7% • • </div> </div>
1	C	274	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 7%, green 7%, green 82%, yellow 82%, yellow 90%, grey 90%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 7% 82% 8% • 9% </div> </div>
2	H	6	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 50%, green 50%, green 67%, yellow 67%, yellow 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 50% 33% 67% </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	TAM	A	501	-	-	X	-
4	DTT	C	401	-	X	-	-
6	GOL	A	507	-	-	X	-
6	GOL	B	406	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6046 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			1995	1249	353	387	6			
1	B	268	Total	C	N	O	S	0	0	0
			2014	1260	357	391	6			
1	C	248	Total	C	N	O	S	0	0	0
			1853	1162	328	356	7			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	initiating methionine	UNP A0A0T9EA39
A	70	ALA	SER	engineered mutation	UNP A0A0T9EA39
A	294	LEU	-	expression tag	UNP A0A0T9EA39
A	295	GLU	-	expression tag	UNP A0A0T9EA39
A	296	HIS	-	expression tag	UNP A0A0T9EA39
A	297	HIS	-	expression tag	UNP A0A0T9EA39
A	298	HIS	-	expression tag	UNP A0A0T9EA39
A	299	HIS	-	expression tag	UNP A0A0T9EA39
A	300	HIS	-	expression tag	UNP A0A0T9EA39
A	301	HIS	-	expression tag	UNP A0A0T9EA39
B	28	MET	-	initiating methionine	UNP A0A0T9EA39
B	70	ALA	SER	engineered mutation	UNP A0A0T9EA39
B	294	LEU	-	expression tag	UNP A0A0T9EA39
B	295	GLU	-	expression tag	UNP A0A0T9EA39
B	296	HIS	-	expression tag	UNP A0A0T9EA39
B	297	HIS	-	expression tag	UNP A0A0T9EA39
B	298	HIS	-	expression tag	UNP A0A0T9EA39
B	299	HIS	-	expression tag	UNP A0A0T9EA39
B	300	HIS	-	expression tag	UNP A0A0T9EA39
B	301	HIS	-	expression tag	UNP A0A0T9EA39
C	28	MET	-	initiating methionine	UNP A0A0T9EA39
C	70	ALA	SER	engineered mutation	UNP A0A0T9EA39
C	294	LEU	-	expression tag	UNP A0A0T9EA39

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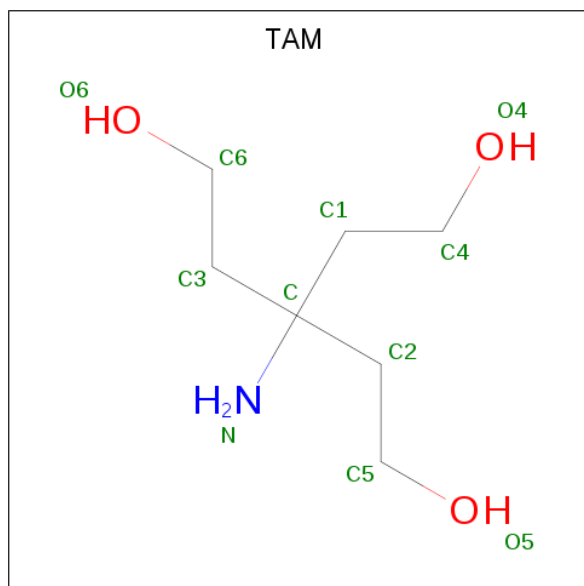
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Chain	Residue	Modelled	Actual	Comment	Reference
C	295	GLU	-	expression tag	UNP A0A0T9EA39
C	296	HIS	-	expression tag	UNP A0A0T9EA39
C	297	HIS	-	expression tag	UNP A0A0T9EA39
C	298	HIS	-	expression tag	UNP A0A0T9EA39
C	299	HIS	-	expression tag	UNP A0A0T9EA39
C	300	HIS	-	expression tag	UNP A0A0T9EA39
C	301	HIS	-	expression tag	UNP A0A0T9EA39

- Molecule 2 is a protein called Possible protein degradation product.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	6	Total	C	N	O	1	0	0
			23	12	5	6			

- Molecule 3 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



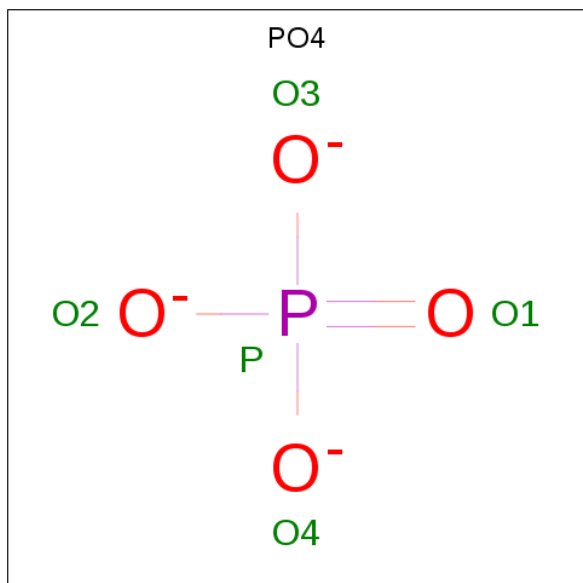
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	7	1	3		
3	A	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



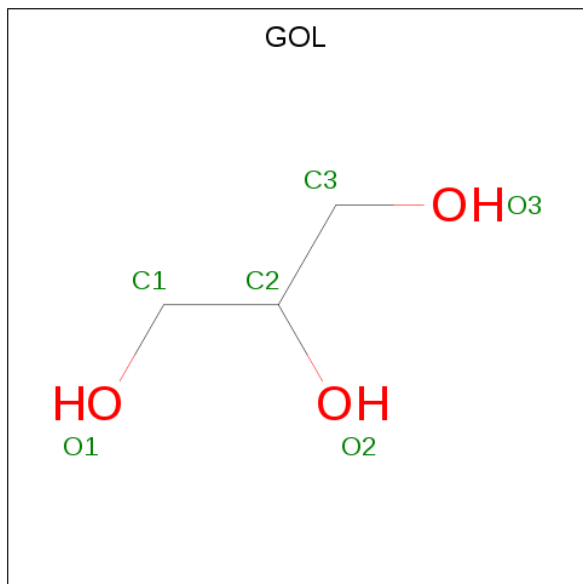
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			8	4	2	2		
4	B	1	Total	C	O	S	0	0
			8	4	2	2		
4	B	1	Total	C	O	S	0	0
			8	4	2	2		
4	C	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	C	1	Total O P 5 4 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

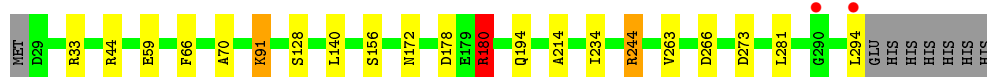
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	25	Total 25	O 25	0	0
7	B	18	Total 18	O 18	0	0
7	C	9	Total 9	O 9	0	0
7	H	1	Total 1	O 1	0	0

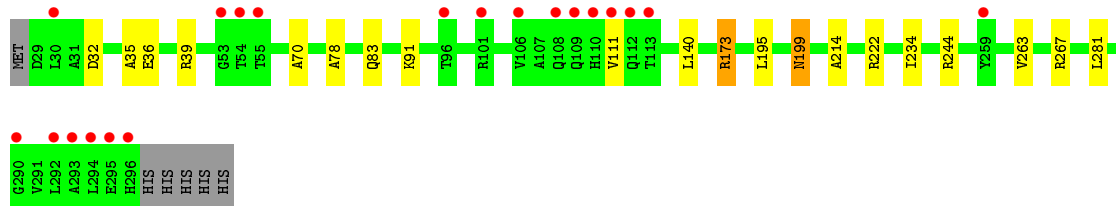
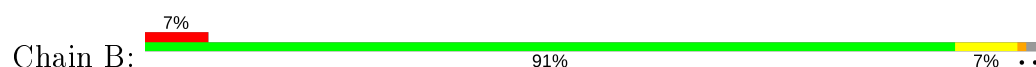
3 Residue-property plots [i](#)

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.

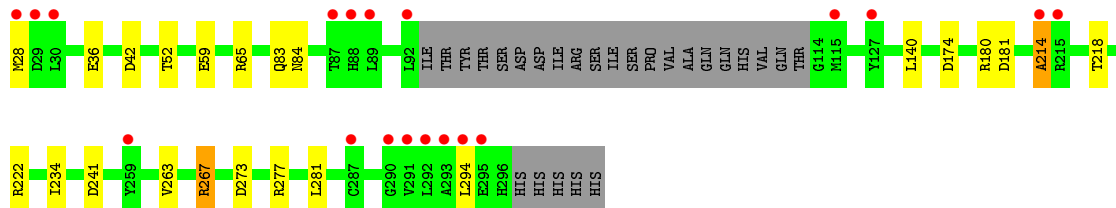
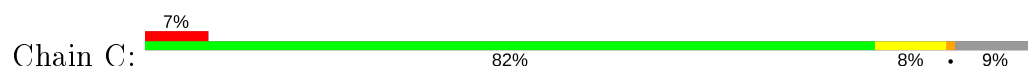
- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



- Molecule 1: Beta-lactamase



- Molecule 2: Possible protein degradation product



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.86Å 108.86Å 260.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 2.54 49.73 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.73-2.54) 99.6 (49.73-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.228 , 0.256 0.233 , 0.259	Depositor DCC
R_{free} test set	2628 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6046	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, DTT, TAM

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	0.69	0/2034	0.90	4/2777 (0.1%)
1	B	0.67	0/2054	0.88	5/2804 (0.2%)
1	C	0.70	0/1889	0.93	8/2575 (0.3%)
2	H	0.92	0/22	1.39	1/26 (3.8%)
All	All	0.69	0/5999	0.91	18/8182 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	273	ASP	CB-CG-OD1	8.65	126.09	118.30
1	A	273	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	C	222	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	C	214	ALA	N-CA-C	6.24	127.85	111.00
1	B	267	ARG	NE-CZ-NH1	-6.14	117.23	120.30
2	H	5	GLY	N-CA-C	-5.87	98.43	113.10
1	A	244	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	273	ASP	CB-CG-OD1	5.75	123.48	118.30
1	C	273	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	B	173	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	A	180	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	C	267	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	C	241	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	222	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	C	65	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	C	65	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	B	244	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	32	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1995	0	1967	16	0
1	B	2014	0	1980	6	0
1	C	1853	0	1822	5	0
2	H	23	0	15	5	0
3	A	22	0	32	8	0
4	A	8	0	10	0	0
4	B	16	0	20	1	0
4	C	8	0	10	0	0
5	A	15	0	0	0	0
5	B	10	0	0	0	0
5	C	5	0	0	0	0
6	A	6	0	8	4	0
6	B	12	0	16	0	0
6	C	6	0	8	1	0
7	A	25	0	0	0	0
7	B	18	0	0	0	0
7	C	9	0	0	0	0
7	H	1	0	0	0	0
All	All	6046	0	5888	30	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 (30) 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:C:52:THR:O	2:H:4:GLY:O	1.62	1.15
1:A:156:SER:OG	2:H:6:GLY:HA2	1.48	1.12
3:A:501:TAM:O6	3:A:501:TAM:N	1.89	1.02
1:A:70:ALA:HB2	3:A:501:TAM:H12	1.51	0.92
1:A:266:ASP:OD2	6:A:507:GOL:H11	2.02	0.59
1:A:214:ALA:HA	1:A:234:ILE:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ALA:CB	3:A:501:TAM:H12	2.31	0.58
1:A:156:SER:OG	2:H:6:GLY:CA	2.38	0.58
1:A:128:SER:OG	3:A:501:TAM:N	2.37	0.57
1:B:214:ALA:HA	1:B:234:ILE:HG22	1.87	0.55
1:A:66:PHE:HA	6:A:507:GOL:H12	1.89	0.54
3:A:501:TAM:H41	3:A:501:TAM:H52	1.90	0.53
1:B:263:VAL:HG12	1:B:281:LEU:HD22	1.92	0.52
1:C:214:ALA:HA	1:C:234:ILE:HG22	1.92	0.51
1:A:263:VAL:HG12	1:A:281:LEU:HD22	1.93	0.51
1:A:156:SER:CB	2:H:6:GLY:HA2	2.40	0.49
1:B:35:ALA:O	1:B:39:ARG:HD3	2.12	0.49
1:A:178:ASP:OD2	1:A:180:ARG:NH2	2.47	0.48
1:A:91:LYS:HG3	3:A:506:TAM:N	2.28	0.48
1:A:194:GLN:HE21	2:H:3:GLY:C	2.17	0.47
1:C:267:ARG:HH12	6:C:403:GOL:H12	1.79	0.47
3:A:501:TAM:C4	3:A:501:TAM:H52	2.46	0.45
1:C:263:VAL:HG12	1:C:281:LEU:HD22	1.98	0.45
1:A:172:ASN:OD1	3:A:501:TAM:C4	2.65	0.45
1:A:244:ARG:HH21	6:A:507:GOL:H2	1.82	0.44
1:B:70:ALA:HB2	4:B:401:DTT:H2	2.00	0.44
1:A:44:ARG:HH11	6:A:507:GOL:H11	1.83	0.44
1:B:199:ASN:HD22	1:B:199:ASN:C	2.23	0.41
1:B:78:ALA:HB1	1:B:195:LEU:HD22	2.03	0.41
1:C:174:ASP:OD2	1:C:181:ASP:OD2	2.40	0.40

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	264/274 (96%)	259 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	266/274 (97%)	258 (97%)	8 (3%)	0	100	100
1	C	244/274 (89%)	234 (96%)	10 (4%)	0	100	100
2	H	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
All	All	778/828 (94%)	754 (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	202/210 (96%)	196 (97%)	6 (3%)	41	55
1	B	204/210 (97%)	197 (97%)	7 (3%)	37	50
1	C	184/210 (88%)	173 (94%)	11 (6%)	19	25
All	All	590/630 (94%)	566 (96%)	24 (4%)	30	41

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	59	GLU
1	A	91	LYS
1	A	140	LEU
1	A	180	ARG
1	A	294	LEU
1	B	36	GLU
1	B	83	GLN
1	B	91	LYS
1	B	111	VAL
1	B	140	LEU
1	B	173	ARG
1	B	199	ASN
1	C	28	MET

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Mol	Chain	Res	Type
1	C	36	GLU
1	C	42	ASP
1	C	59	GLU
1	C	83	GLN
1	C	84	ASN
1	C	140	LEU
1	C	180	ARG
1	C	218	THR
1	C	277	ARG
1	C	294	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	194	GLN
1	B	109	GLN
1	B	199	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 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
6	GOL	C	403	-	5,5,5	0.70	0	5,5,5	1.01	0
6	GOL	B	406	-	5,5,5	2.00	2 (40%)	5,5,5	0.83	0
4	DTT	B	401	-	7,7,7	1.46	1 (14%)	4,8,8	1.64	1 (25%)
4	DTT	A	502	-	7,7,7	1.08	0	4,8,8	1.68	1 (25%)
5	PO4	C	402	-	4,4,4	1.01	0	6,6,6	0.78	0
3	TAM	A	501	5	7,10,10	1.18	0	9,12,12	2.24	3 (33%)
4	DTT	B	402	-	7,7,7	0.96	0	4,8,8	3.00	2 (50%)
5	PO4	A	503	-	4,4,4	0.60	0	6,6,6	1.63	2 (33%)
3	TAM	A	506	-	7,10,10	1.21	1 (14%)	9,12,12	0.84	0
6	GOL	A	507	-	5,5,5	1.33	1 (20%)	5,5,5	1.24	0
5	PO4	A	504	-	4,4,4	0.89	0	6,6,6	0.49	0
5	PO4	A	505	3	4,4,4	0.48	0	6,6,6	1.44	1 (16%)
5	PO4	B	403	-	4,4,4	0.74	0	6,6,6	1.12	0
4	DTT	C	401	-	7,7,7	1.45	2 (28%)	4,8,8	2.88	1 (25%)
5	PO4	B	404	-	4,4,4	0.84	0	6,6,6	1.27	1 (16%)
6	GOL	B	405	-	5,5,5	0.80	0	5,5,5	0.81	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
6	GOL	C	403	-	-	2/4/4/4	-
4	DTT	B	401	-	-	4/8/8/8	-
4	DTT	A	502	-	-	6/8/8/8	-
6	GOL	B	406	-	-	4/4/4/4	-
3	TAM	A	501	5	-	8/12/12/12	-
4	DTT	B	402	-	-	2/8/8/8	-
3	TAM	A	506	-	-	5/12/12/12	-
6	GOL	A	507	-	-	4/4/4/4	-
4	DTT	C	401	-	-	7/8/8/8	-
6	GOL	B	405	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	406	GOL	O1-C1	2.71	1.53	1.42
4	C	401	DTT	O3-C3	2.38	1.48	1.43
6	A	507	GOL	O2-C2	2.13	1.49	1.43
4	C	401	DTT	C3-C2	2.12	1.58	1.52
3	A	506	TAM	C3-C6	2.08	1.56	1.52
4	B	401	DTT	C4-S4	-2.05	1.77	1.81
6	B	406	GOL	O3-C3	2.00	1.50	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	DTT	O3-C3-C2	5.32	120.66	109.72
3	A	501	TAM	C2-C-C1	4.45	118.36	110.50
4	B	402	DTT	O2-C2-C3	-4.26	100.98	109.72
4	B	402	DTT	C2-C1-S1	4.23	126.76	114.47
3	A	501	TAM	C3-C-N	-3.35	98.55	108.09
5	A	503	PO4	O4-P-O2	3.18	118.19	107.97
4	B	401	DTT	O3-C3-C2	2.90	115.68	109.72
4	A	502	DTT	O3-C3-C2	2.80	115.47	109.72
5	A	505	PO4	O2-P-O1	-2.54	101.58	110.89
3	A	501	TAM	C1-C-N	-2.13	102.03	108.09
5	A	503	PO4	O3-P-O2	-2.06	101.37	107.97
5	B	404	PO4	O4-P-O3	-2.05	101.38	107.97

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	403	GOL	C1-C2-C3-O3
4	B	401	DTT	S1-C1-C2-O2
4	B	401	DTT	S1-C1-C2-C3
4	B	401	DTT	C2-C3-C4-S4
4	B	401	DTT	O3-C3-C4-S4
4	A	502	DTT	C1-C2-C3-O3
4	A	502	DTT	C1-C2-C3-C4
4	A	502	DTT	O2-C2-C3-O3
4	A	502	DTT	O2-C2-C3-C4
4	A	502	DTT	C2-C3-C4-S4
4	A	502	DTT	O3-C3-C4-S4
3	A	501	TAM	C3-C-C1-C4
3	A	501	TAM	C1-C-C2-C5

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Mol	Chain	Res	Type	Atoms
3	A	501	TAM	C3-C-C2-C5
3	A	501	TAM	N-C-C2-C5
3	A	501	TAM	C2-C-C3-C6
3	A	501	TAM	N-C-C3-C6
3	A	501	TAM	C-C1-C4-O4
4	B	402	DTT	S1-C1-C2-O2
4	B	402	DTT	S1-C1-C2-C3
3	A	506	TAM	C1-C-C3-C6
3	A	506	TAM	C2-C-C3-C6
3	A	506	TAM	N-C-C3-C6
6	A	507	GOL	O1-C1-C2-C3
4	C	401	DTT	S1-C1-C2-O2
4	C	401	DTT	S1-C1-C2-C3
4	C	401	DTT	C1-C2-C3-O3
4	C	401	DTT	C1-C2-C3-C4
4	C	401	DTT	O2-C2-C3-O3
4	C	401	DTT	O2-C2-C3-C4
6	B	405	GOL	C1-C2-C3-O3
6	C	403	GOL	O2-C2-C3-O3
6	B	406	GOL	O1-C1-C2-C3
6	B	406	GOL	C1-C2-C3-O3
6	A	507	GOL	C1-C2-C3-O3
6	B	406	GOL	O2-C2-C3-O3
6	A	507	GOL	O2-C2-C3-O3
3	A	501	TAM	C-C3-C6-O6
3	A	506	TAM	C-C1-C4-O4
6	B	405	GOL	O2-C2-C3-O3
6	B	406	GOL	O1-C1-C2-O2
4	C	401	DTT	O3-C3-C4-S4
3	A	506	TAM	C-C3-C6-O6
6	A	507	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	403	GOL	1	0
4	B	401	DTT	1	0
3	A	501	TAM	7	0
3	A	506	TAM	1	0
6	A	507	GOL	4	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, 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	266/274 (97%)	-0.05	2 (0%) 86 89	43, 55, 78, 97	0
1	B	268/274 (97%)	0.23	20 (7%) 14 17	46, 61, 93, 129	0
1	C	248/274 (90%)	0.30	19 (7%) 13 17	45, 65, 107, 133	0
2	H	6/6 (100%)	2.80	3 (50%) 0 0	80, 94, 101, 104	1 (16%)
All	All	788/828 (95%)	0.17	44 (5%) 24 29	43, 60, 95, 133	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	6	GLY	6.1
1	B	294	LEU	5.8
2	H	4	GLY	5.7
1	C	295	GLU	5.5
1	C	87	THR	4.0
1	C	291	VAL	4.0
1	B	259	TYR	3.9
1	B	109	GLN	3.9
1	C	28	MET	3.8
1	B	108	GLN	3.7
1	B	54	THR	3.5
1	C	294	LEU	3.3
1	C	292	LEU	3.2
1	B	113	THR	3.2
1	B	292	LEU	3.1
1	C	293	ALA	3.1
1	C	290	GLY	3.0
1	B	111	VAL	3.0
1	B	30	LEU	2.9
1	B	293	ALA	2.9
1	C	92	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	215	ARG	2.8
1	B	106	VAL	2.7
1	A	294	LEU	2.7
1	B	112	GLN	2.6
1	C	29	ASP	2.6
1	B	101	ARG	2.6
1	C	30	LEU	2.5
1	C	115	MET	2.4
1	C	287	CYS	2.3
1	C	127	TYR	2.3
1	B	55	THR	2.3
1	C	259	TYR	2.3
1	B	96	THR	2.2
1	B	110	HIS	2.2
1	B	295	GLU	2.2
1	C	88	HIS	2.2
1	B	53	GLY	2.1
1	B	296	HIS	2.1
1	C	89	LEU	2.1
1	C	214	ALA	2.1
2	H	7	GLY	2.1
1	B	290	GLY	2.0
1	A	290	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	B	405	6/6	0.73	0.14	83,88,98,99	0
6	GOL	A	507	6/6	0.75	0.24	58,74,81,85	0
3	TAM	A	506	11/11	0.76	0.18	71,102,122,123	0
6	GOL	B	406	6/6	0.80	0.19	56,64,69,71	0
6	GOL	C	403	6/6	0.85	0.22	60,77,80,81	0
4	DTT	A	502	8/8	0.86	0.24	87,108,110,113	0
4	DTT	C	401	8/8	0.87	0.19	74,93,98,101	0
5	PO4	C	402	5/5	0.88	0.21	90,101,121,124	0
4	DTT	B	402	8/8	0.88	0.17	76,95,100,102	0
5	PO4	B	404	5/5	0.89	0.20	50,53,63,68	5
5	PO4	A	504	5/5	0.90	0.20	77,113,127,129	0
3	TAM	A	501	11/11	0.91	0.23	51,75,84,86	2
5	PO4	B	403	5/5	0.94	0.12	82,83,86,94	0
5	PO4	A	503	5/5	0.94	0.19	71,77,88,97	0
4	DTT	B	401	8/8	0.94	0.15	56,80,84,88	0
5	PO4	A	505	5/5	0.94	0.31	46,59,66,70	5

6.5 Other polymers [i](#)

There are no such residues in this entry.