



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2017 – 08:02 PM EST

PDB ID : 4X7M
Title : Crystal structure of *S. aureus* TarM G117R mutant in complex with UDP and UDP-GlcNAc
Authors : Worrall, L.J.; Sobhanifar, S.; Strynadka, N.C.
Deposited on : unknown
Resolution : 2.40 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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

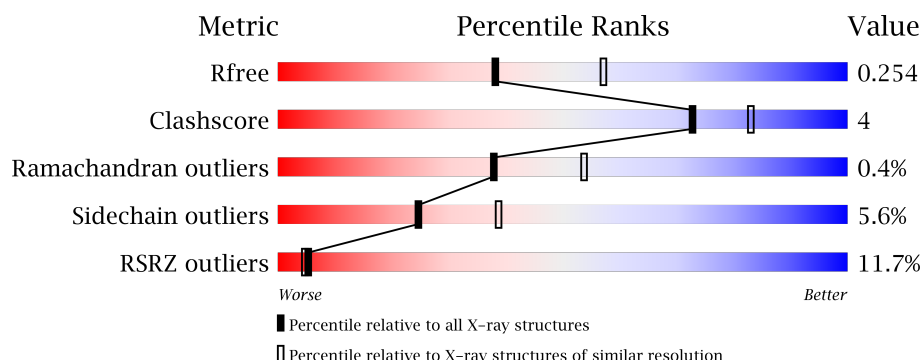
1 Overall quality at a glance

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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (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 ≥ 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	493	<div> <div>4%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	B	493	<div> <div>19%</div> <div>86%</div> <div>14%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8181 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.

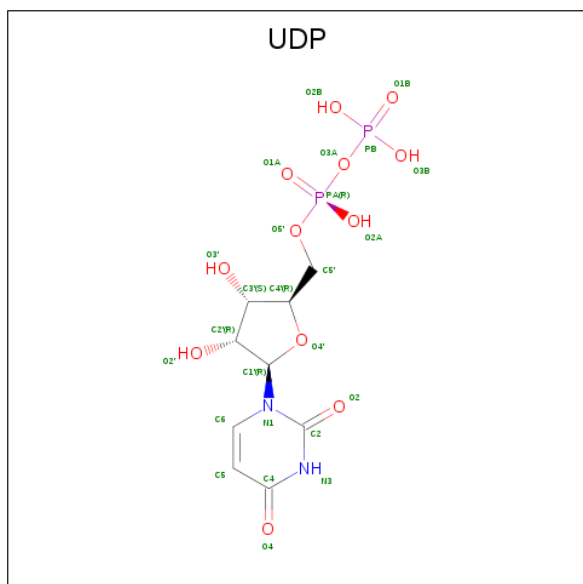
- Molecule 1 is a protein called TarM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			4024	2573	680	752	19			
1	B	493	Total	C	N	O	S	0	0	0
			4034	2582	681	752	19			

There are 2 discrepancies between the modelled and reference sequences:

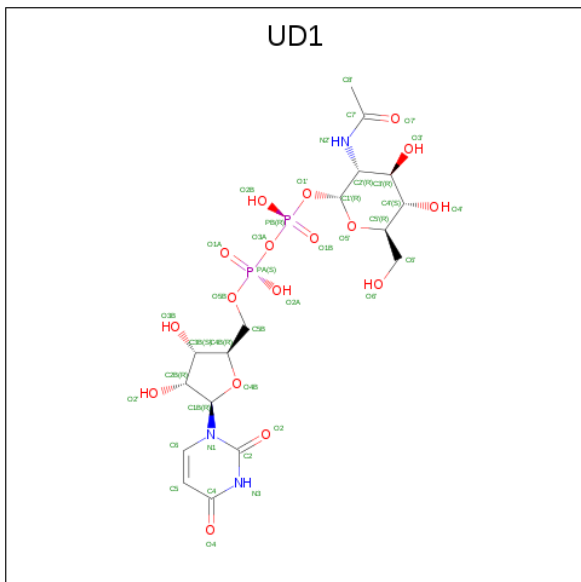
Chain	Residue	Modelled	Actual	Comment	Reference
A	117	ARG	GLY	engineered mutation	UNP H0AM96
B	117	ARG	GLY	engineered mutation	UNP H0AM96

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

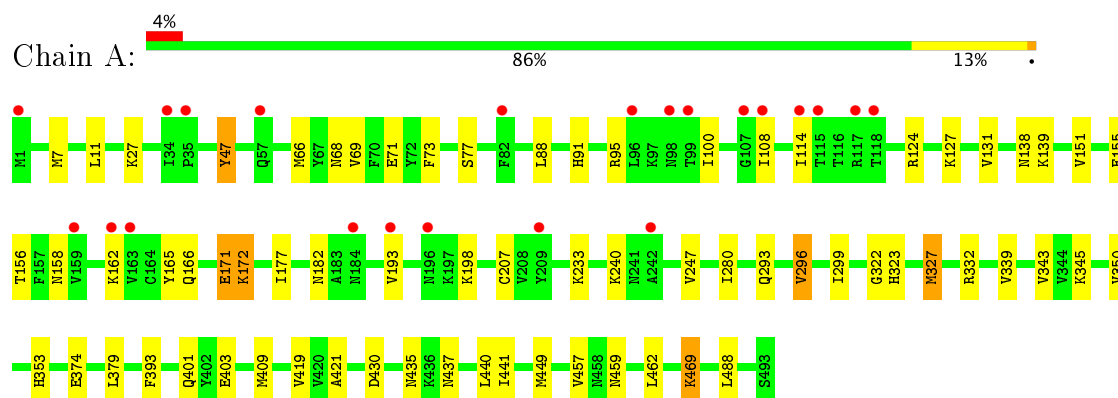
- Molecule 3 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).



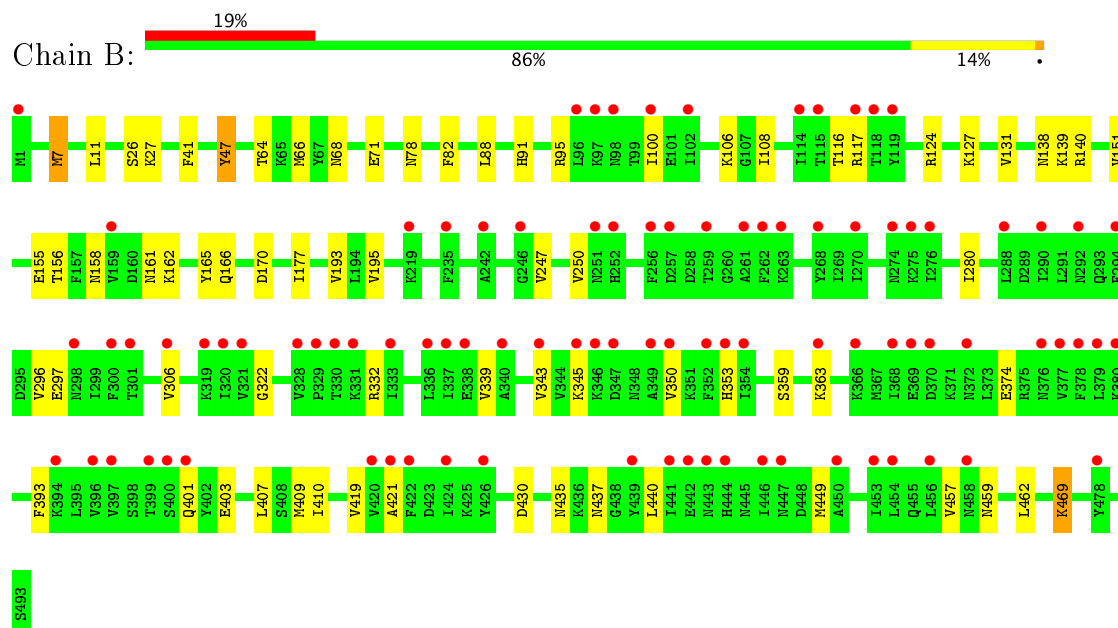
3 Residue-property plots [i](#)

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: TarM



• Molecule 1: TarM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	44.07Å 90.94Å 94.44Å 109.27° 99.03° 101.53°	Depositor
Resolution (Å)	46.04 – 2.40 46.04 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.3 (46.04-2.40) 82.8 (46.04-2.40)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.39Å)	Xtriage
Refinement program	BUSTER, REFMAC	Depositor
R, R_{free}	0.233 , 0.274 0.251 , 0.254	Depositor DCC
R_{free} test set	2501 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8181	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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: UDP, UD1

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	0.51	0/4100	0.71	0/5505
1	B	0.49	0/4111	0.72	0/5518
All	All	0.50	0/8211	0.71	0/11023

There are no bond length outliers.

There are no bond angle outliers.

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	4024	0	4038	30	0
1	B	4034	0	4056	34	0
2	A	25	0	11	0	0
3	B	39	0	25	4	0
4	A	37	0	0	3	0
4	B	22	0	0	1	0
All	All	8181	0	8130	64	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 4.

All (64) 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:88:LEU:CD2	1:B:151:VAL:HG11	2.16	0.74
1:B:250:VAL:HG12	3:B:501:UD1:H8'3	1.67	0.74
1:B:88:LEU:HD23	1:B:151:VAL:HG11	1.69	0.73
1:A:343:VAL:HG12	1:A:350:VAL:HG11	1.70	0.73
1:B:64:THR:HG21	4:B:608:HOH:O	1.90	0.71
1:B:343:VAL:HG12	1:B:350:VAL:HG11	1.71	0.71
1:A:332:ARG:HG3	1:A:401:GLN:HG2	1.79	0.64
1:B:332:ARG:HG3	1:B:401:GLN:HG2	1.80	0.63
1:B:403:GLU:HG3	3:B:501:UD1:O3'	2.01	0.60
1:A:156:THR:HB	1:A:165:TYR:HB3	1.84	0.59
1:B:156:THR:HB	1:B:165:TYR:HB3	1.85	0.58
1:A:296:VAL:HG12	1:A:299:ILE:HD11	1.87	0.57
1:B:11:LEU:HD12	1:B:66:MET:HE3	1.87	0.56
1:B:177:ILE:HG12	1:B:193:VAL:HG12	1.87	0.56
1:B:7:MET:HG2	1:B:41:PHE:HZ	1.72	0.54
1:A:403:GLU:HG3	4:A:637:HOH:O	2.08	0.53
1:A:68:ASN:HB3	1:A:71:GLU:HB2	1.89	0.53
1:A:108:ILE:HG12	1:A:124:ARG:HG3	1.90	0.53
1:A:339:VAL:HG21	1:A:449:MET:HE2	1.90	0.53
1:A:177:ILE:HG12	1:A:193:VAL:HG12	1.91	0.53
1:B:108:ILE:HG12	1:B:124:ARG:HG3	1.90	0.53
1:B:140:ARG:HD2	1:B:161:ASN:OD1	2.10	0.52
1:B:403:GLU:HG3	3:B:501:UD1:HO3'	1.76	0.51
1:B:306:VAL:HG11	1:B:410:ILE:HG21	1.94	0.50
1:B:339:VAL:HG21	1:B:449:MET:HE2	1.93	0.50
1:A:207:CYS:HB2	1:A:233:LYS:HG2	1.93	0.49
1:A:171:GLU:HG3	1:A:172:LYS:HD2	1.95	0.49
1:A:11:LEU:HB2	1:A:66:MET:HE2	1.95	0.49
1:A:323:HIS:HE1	4:A:609:HOH:O	1.96	0.48
1:B:403:GLU:HA	3:B:501:UD1:H8'2	1.94	0.48
1:B:7:MET:HG2	1:B:41:PHE:CZ	2.48	0.48
1:B:247:VAL:HG13	1:B:280:ILE:HG22	1.96	0.48
1:A:11:LEU:HD12	1:A:66:MET:HE3	1.96	0.47
1:B:68:ASN:HB3	1:B:71:GLU:HB2	1.95	0.47
1:A:158:ASN:HD21	1:A:162:LYS:HB2	1.78	0.47
1:A:293:GLN:HG2	4:A:606:HOH:O	2.13	0.47
1:B:78:ASN:OD1	1:B:170:ASP:HB2	2.14	0.47
1:B:155:GLU:HG2	1:B:166:GLN:HG2	1.97	0.47
1:A:88:LEU:HD23	1:A:151:VAL:HG11	1.95	0.47
1:B:437:ASN:HB3	1:B:469:LYS:HB3	1.97	0.47
1:B:158:ASN:HD21	1:B:162:LYS:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:HIS:O	1:A:95:ARG:HG2	2.17	0.45
1:B:26:SER:OG	1:B:64:THR:HB	2.16	0.45
1:B:339:VAL:HG11	1:B:449:MET:HE3	1.99	0.45
1:A:437:ASN:HB3	1:A:469:LYS:HB3	1.99	0.45
1:A:155:GLU:HG2	1:A:166:GLN:HG2	2.00	0.44
1:A:322:GLY:HA3	1:A:393:PHE:CD2	2.52	0.44
1:A:247:VAL:HG13	1:A:280:ILE:HG22	2.00	0.44
1:B:322:GLY:HA3	1:B:393:PHE:CD2	2.53	0.44
1:A:327:MET:HE3	1:A:379:LEU:HD22	1.99	0.43
1:A:88:LEU:CD2	1:A:151:VAL:HG11	2.49	0.43
1:B:91:HIS:O	1:B:95:ARG:HG2	2.19	0.43
1:A:409:MET:HE2	1:A:419:VAL:HG11	2.01	0.42
1:A:47:TYR:CE1	1:A:66:MET:HE1	2.55	0.42
1:B:332:ARG:CG	1:B:401:GLN:HG2	2.47	0.42
1:A:339:VAL:HG11	1:A:449:MET:HE3	2.02	0.42
1:B:47:TYR:CE1	1:B:66:MET:HE1	2.55	0.42
1:B:11:LEU:HB2	1:B:66:MET:HE2	2.02	0.41
1:A:69:VAL:O	1:A:73:PHE:HD2	2.03	0.41
1:B:409:MET:HE2	1:B:419:VAL:HG11	2.02	0.41
1:A:409:MET:HE3	1:A:421:ALA:CB	2.50	0.40
1:B:409:MET:HE3	1:B:421:ALA:CB	2.52	0.40
1:A:441:ILE:HG21	1:A:449:MET:HB2	2.04	0.40
1:B:116:THR:O	1:B:117:ARG:CB	2.69	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	491/493 (100%)	465 (95%)	25 (5%)	1 (0%)	51 67
1	B	491/493 (100%)	470 (96%)	18 (4%)	3 (1%)	28 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	982/986 (100%)	935 (95%)	43 (4%)	4 (0%)	38 54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	407	LEU
1	A	127	LYS
1	B	127	LYS
1	B	359	SER

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	447/450 (99%)	420 (94%)	27 (6%)	22 35
1	B	449/450 (100%)	426 (95%)	23 (5%)	28 44
All	All	896/900 (100%)	846 (94%)	50 (6%)	25 39

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	MET
1	A	27	LYS
1	A	47	TYR
1	A	77	SER
1	A	100	ILE
1	A	114	ILE
1	A	131	VAL
1	A	138	ASN
1	A	139	LYS
1	A	171	GLU
1	A	172	LYS
1	A	182	ASN
1	A	198	LYS
1	A	240	LYS

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Mol	Chain	Res	Type
1	A	296	VAL
1	A	327	MET
1	A	345	LYS
1	A	353	HIS
1	A	374	GLU
1	A	430	ASP
1	A	435	ASN
1	A	440	LEU
1	A	457	VAL
1	A	459	ASN
1	A	462	LEU
1	A	469	LYS
1	A	488	LEU
1	B	7	MET
1	B	27	LYS
1	B	47	TYR
1	B	82	PHE
1	B	100	ILE
1	B	106	LYS
1	B	131	VAL
1	B	138	ASN
1	B	139	LYS
1	B	195	VAL
1	B	296	VAL
1	B	297	GLU
1	B	345	LYS
1	B	353	HIS
1	B	363	LYS
1	B	374	GLU
1	B	430	ASP
1	B	435	ASN
1	B	440	LEU
1	B	457	VAL
1	B	459	ASN
1	B	462	LEU
1	B	469	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	196	ASN

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Mol	Chain	Res	Type
1	A	323	HIS
1	A	459	ASN
1	B	182	ASN
1	B	241	ASN
1	B	459	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](#)

2 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	UDP	A	500	-	21,26,26	1.08	2 (9%)	22,40,40	3.34	2 (9%)
3	UD1	B	501	-	34,41,41	1.84	7 (20%)	43,62,62	1.73	8 (18%)

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	UDP	A	500	-	-	0/12/32/32	0/2/2/2
3	UD1	B	501	-	-	0/22/63/63	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	UD1	C2'-N2'	2.00	1.49	1.45
3	B	501	UD1	PB-O1'	2.02	1.65	1.60
2	A	500	UDP	C6-N1	2.40	1.39	1.35
3	B	501	UD1	C1'-C2'	2.42	1.57	1.53
3	B	501	UD1	O5'-C1'	2.77	1.48	1.41
3	B	501	UD1	C3'-C2'	2.97	1.59	1.53
2	A	500	UDP	C4-N3	3.38	1.39	1.33
3	B	501	UD1	C4-N3	4.85	1.41	1.33
3	B	501	UD1	C6-N1	5.83	1.43	1.35

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	UDP	C5-C4-N3	-3.53	114.69	123.12
3	B	501	UD1	O4B-C4B-C5B	-3.27	98.36	109.40
3	B	501	UD1	C4B-O4B-C1B	-2.92	106.66	109.77
3	B	501	UD1	O5'-C1'-O1'	-2.82	107.69	111.36
3	B	501	UD1	C2'-N2'-C7'	2.03	128.34	123.19
3	B	501	UD1	C1'-O5'-C5'	2.13	117.74	113.72
3	B	501	UD1	PB-O1'-C1'	2.49	129.61	119.74
3	B	501	UD1	O1'-C1'-C2'	2.50	112.93	108.40
3	B	501	UD1	C4-N3-C2	7.47	120.55	114.13
2	A	500	UDP	C4-N3-C2	15.04	127.05	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	UD1	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	493/493 (100%)	0.22	22 (4%) 34 32	33, 78, 131, 154	0
1	B	493/493 (100%)	0.88	93 (18%) 1 1	34, 94, 161, 193	0
All	All	986/986 (100%)	0.55	115 (11%) 5 5	33, 85, 147, 193	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	368	ILE	10.9
1	B	444	HIS	8.0
1	B	262	PHE	7.2
1	B	370	ASP	7.0
1	B	378	PHE	7.0
1	B	345	LYS	6.8
1	B	343	VAL	6.8
1	B	443	ASN	6.2
1	B	270	ILE	6.2
1	B	366	LYS	6.0
1	B	114	ILE	5.6
1	B	319	LYS	5.6
1	B	447	ASN	5.3
1	B	340	ALA	5.0
1	B	354	ILE	5.0
1	B	336	LEU	4.9
1	B	376	ASN	4.8
1	B	338	GLU	4.8
1	B	439	TYR	4.6
1	A	82	PHE	4.6
1	B	276	ILE	4.3
1	B	329	PRO	4.3
1	B	320	ILE	4.3
1	B	347	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	400	SER	4.2
1	B	442	GLU	4.2
1	B	369	GLU	4.1
1	B	331	LYS	4.1
1	B	397	VAL	4.1
1	B	377	VAL	3.8
1	A	99	THR	3.8
1	B	333	ILE	3.8
1	B	263	LYS	3.7
1	B	454	LEU	3.6
1	B	159	VAL	3.5
1	B	401	GLN	3.5
1	A	115	THR	3.5
1	B	292	ASN	3.4
1	B	420	VAL	3.4
1	A	96	LEU	3.4
1	B	330	THR	3.4
1	B	321	VAL	3.3
1	B	115	THR	3.3
1	B	453	ILE	3.3
1	A	117	ARG	3.2
1	B	1	MET	3.2
1	B	379	LEU	3.2
1	B	290	ILE	3.2
1	B	372	ASN	3.1
1	B	246	GLY	3.0
1	B	426	TYR	3.0
1	B	256	PHE	3.0
1	B	294	PHE	3.0
1	B	261	ALA	2.9
1	B	251	ASN	2.9
1	B	268	TYR	2.9
1	B	298	ASN	2.9
1	B	394	LYS	2.9
1	B	352	PHE	2.9
1	B	422	PHE	2.8
1	A	114	ILE	2.8
1	B	350	VAL	2.7
1	B	288	LEU	2.7
1	B	346	LYS	2.7
1	A	184	ASN	2.7
1	A	242	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	257	ASP	2.7
1	B	97	LYS	2.7
1	B	306	VAL	2.7
1	B	337	ILE	2.7
1	B	96	LEU	2.7
1	B	252	HIS	2.6
1	B	380	LYS	2.6
1	A	163	VAL	2.6
1	B	275	LYS	2.5
1	A	98	ASN	2.5
1	B	274	ASN	2.5
1	B	300	PHE	2.5
1	B	117	ARG	2.5
1	B	328	VAL	2.5
1	B	353	HIS	2.5
1	B	118	THR	2.5
1	B	446	ILE	2.4
1	A	35	PRO	2.4
1	B	219	LYS	2.4
1	B	424	ILE	2.4
1	B	242	ALA	2.4
1	B	456	LEU	2.4
1	B	450	ALA	2.4
1	B	399	THR	2.4
1	B	102	ILE	2.4
1	A	209	TYR	2.4
1	B	235	PHE	2.3
1	A	196	ASN	2.3
1	B	259	THR	2.3
1	A	1	MET	2.2
1	A	108	ILE	2.2
1	B	421	ALA	2.2
1	A	57	GLN	2.2
1	B	100	ILE	2.2
1	B	98	ASN	2.2
1	B	441	ILE	2.2
1	A	162	LYS	2.2
1	B	478	TYR	2.2
1	A	34	ILE	2.1
1	B	349	ALA	2.1
1	A	193	VAL	2.1
1	B	119	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	107	GLY	2.1
1	B	301	THR	2.0
1	B	396	VAL	2.0
1	A	159	VAL	2.0
1	B	363	LYS	2.0
1	B	458	ASN	2.0
1	A	118	THR	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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	UD1	B	501	39/39	0.93	0.17	-0.40	61,70,91,94	0
2	UDP	A	500	25/25	0.96	0.12	-0.61	52,62,71,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.