WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:13 PM GMT

PDB ID	:	1NZC
Title	:	The high resolution structures of RmlC from Streptococcus suis in complex with dTDP-D-xylose
Authors	:	Dong, C.; Major, L.L.; Allen, A.; Blankenfeldt, W.; Maskell, D.; Naismith, J.H.
Deposited on	:	2003-02-17
Resolution	:	1.80 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

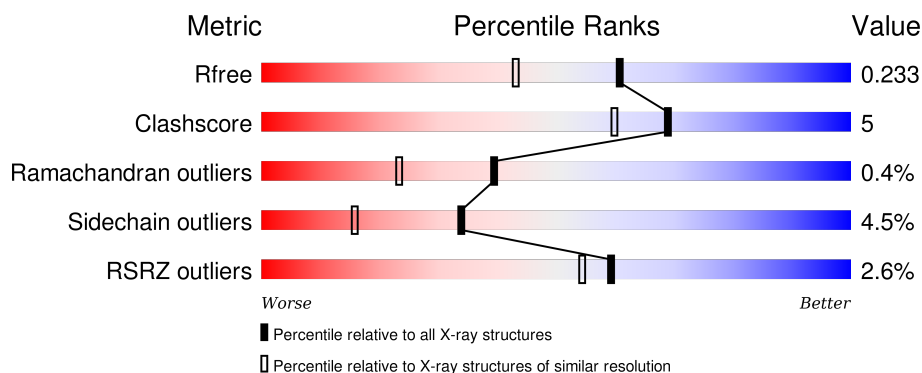|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	Percentile Ranks	Value
Rfree		0.233
Clashscore		5
Ramachandran outliers		0.4%
Sidechain outliers		4.5%
RSRZ outliers		2.6%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 <=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	197	% 86% 11% •••
1	B	197	7% 82% 15% •••
1	C	197	% 86% 11% •••
1	D	197	% 86% 11% ••

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TDX	B	9001	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7316 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.
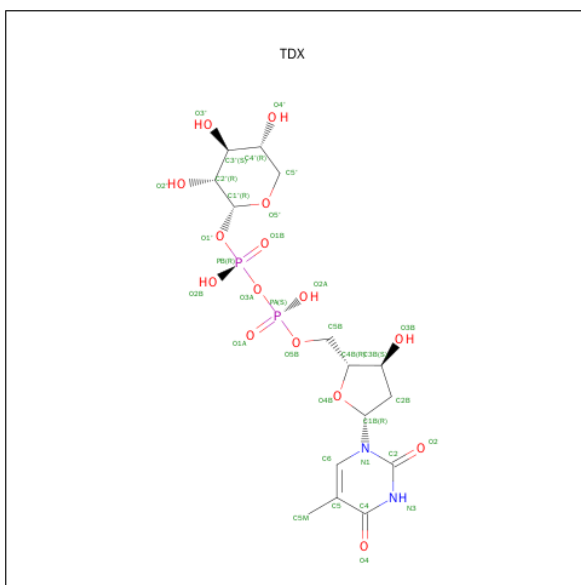
- Molecule 1 is a protein called dTDP-6-deoxy-D-xylo-4-hexulose 3,5-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1584	1026	259	297	2			
1	B	196	Total	C	N	O	S	0	0	0
			1584	1026	259	297	2			
1	C	194	Total	C	N	O	S	0	0	0
			1568	1017	257	292	2			
1	D	194	Total	C	N	O	S	0	0	0
			1568	1017	257	292	2			

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ni	0	0
			1	1		
2	C	1	Total	Ni	0	0
			1	1		

- Molecule 3 is THYMIDINE-5'-DIPHOSPHO-BETA-D-XYLOSE (three-letter code: TDX) (formula: $C_{15}H_{24}N_2O_{15}P_2$).

TDX

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	1	0
			34	15	2	15	2		
3	A	1	Total	C	N	O	P	0	0
			34	15	2	15	2		
3	C	1	Total	C	N	O	P	0	0
			34	15	2	15	2		
3	D	1	Total	C	N	O	P	0	0
			34	15	2	15	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	225	Total	O	0	0
			225	225		
4	B	198	Total	O	0	0
			198	198		
4	C	246	Total	O	0	0
			246	246		
4	D	205	Total	O	0	0
			205	205		

3 Residue-property plots ⓘ

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.
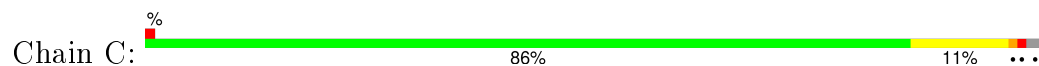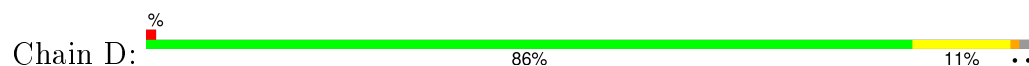
- Molecule 1: dTDP-6-deoxy-D-xylo-4-hexulose 3,5-epimerase
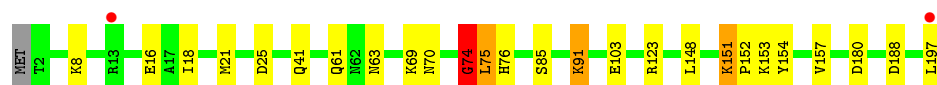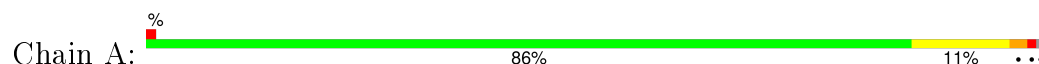
- Molecule 1: dTDP-6-deoxy-D-xylo-4-hexulose 3,5-epimerase
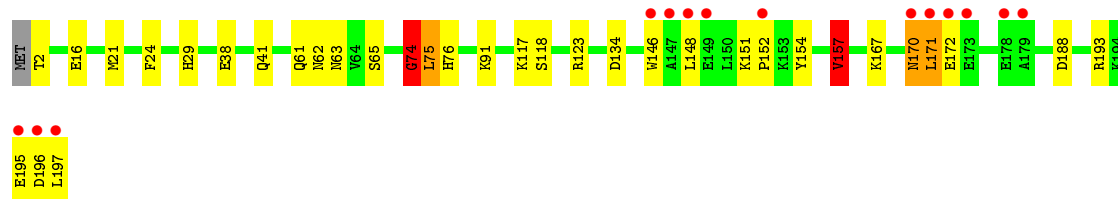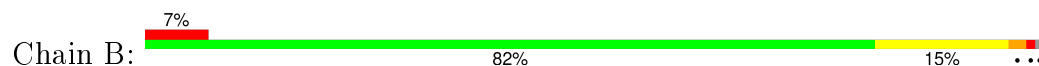
- Molecule 1: dTDP-6-deoxy-D-xylo-4-hexulose 3,5-epimerase

- Molecule 1: dTDP-6-deoxy-D-xylo-4-hexulose 3,5-epimerase

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.85Å 140.87Å 53.70Å 90.00° 92.72° 90.00°	Depositor
Resolution (Å)	70.71 – 1.80 50.79 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.8 (70.71-1.80) 91.8 (50.79-1.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	4.44 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.164 , 0.216 0.193 , 0.233	Depositor DCC
R_{free} test set	3217 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.3	EDS
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 63933 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7316	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: NI, TDX

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	0.61	0/1629	0.82	5/2209 (0.2%)
1	B	0.67	2/1629 (0.1%)	0.87	4/2209 (0.2%)
1	C	0.63	0/1613	0.82	5/2187 (0.2%)
1	D	0.59	0/1613	0.85	9/2187 (0.4%)
All	All	0.63	2/6484 (0.0%)	0.84	23/8792 (0.3%)

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	2
1	B	0	1
1	C	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	ASN	CG-ND2	-5.74	1.18	1.32
1	B	62	ASN	CG-OD1	-5.16	1.12	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	GLY	CA-C-N	-7.54	100.60	117.20
1	D	74	GLY	CA-C-N	-7.32	101.10	117.20
1	B	188	ASP	CB-CG-OD2	7.26	124.83	118.30
1	D	74	GLY	O-C-N	7.15	134.14	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	74	GLY	CA-C-N	-6.85	102.13	117.20
1	D	74	GLY	C-N-CA	6.82	138.76	121.70
1	C	74	GLY	O-C-N	6.50	133.10	122.70
1	A	74	GLY	C-N-CA	6.40	137.70	121.70
1	D	188	ASP	CB-CG-OD2	6.28	123.95	118.30
1	C	74	GLY	C-N-CA	6.27	137.38	121.70
1	D	75	LEU	CB-CA-C	6.24	122.06	110.20
1	A	74	GLY	O-C-N	6.18	132.58	122.70
1	A	188	ASP	CB-CG-OD2	5.94	123.64	118.30
1	C	75	LEU	CB-CA-C	5.93	121.47	110.20
1	D	196	ASP	CB-CG-OD2	5.56	123.31	118.30
1	D	180	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	180	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	81	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	134	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	74	GLY	N-CA-C	5.33	126.41	113.10
1	B	157	VAL	CB-CA-C	-5.27	101.39	111.40
1	C	180	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	74	GLY	CA-C-N	-5.11	105.96	117.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	74	GLY	Mainchain,Peptide
1	B	74	GLY	Peptide
1	C	74	GLY	Peptide

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	1584	0	1525	17	1
1	B	1584	0	1525	17	2
1	C	1568	0	1512	16	0
1	D	1568	0	1512	10	0
2	B	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
3	A	34	0	22	0	0
3	B	34	0	22	0	0
3	C	34	0	22	1	0
3	D	34	0	22	0	0
4	A	225	0	0	8	6
4	B	198	0	0	6	2
4	C	246	0	0	3	4
4	D	205	0	0	0	1
All	All	7316	0	6162	58	8

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 5.

All (58) 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:61:GLN:HE21	1:C:63:ASN:HD21	1.08	0.99
1:D:61:GLN:HE21	1:D:63:ASN:HD21	1.15	0.94
1:B:61:GLN:HE21	1:B:63:ASN:HD21	1.07	0.93
1:B:196:ASP:OD2	4:B:9634:HOH:O	1.87	0.92
1:A:61:GLN:HE21	1:A:63:ASN:HD21	1.18	0.89
1:A:85:SER:OG	4:A:9077:HOH:O	1.58	0.82
1:B:76:HIS:ND1	4:B:9636:HOH:O	2.04	0.80
2:B:9603:NI:NI	4:B:9656:HOH:O	1.28	0.75
1:D:74:GLY:HA2	1:D:76:HIS:CE1	2.23	0.74
1:C:197:LEU:HD23	4:C:9813:HOH:O	1.89	0.71
1:D:46:LEU:HD23	1:D:50:PHE:O	1.92	0.69
1:B:170:ASN:O	1:B:172:GLU:N	2.27	0.67
1:C:74:GLY:HA2	1:C:76:HIS:CE1	2.29	0.67
1:A:197:LEU:HA	4:A:9121:HOH:O	1.95	0.66
1:A:123:ARG:HD3	4:A:9074:HOH:O	1.95	0.66
1:A:74:GLY:HA2	1:A:76:HIS:CE1	2.31	0.65
1:A:91:LYS:HG2	4:A:9003:HOH:O	1.99	0.63
1:B:151:LYS:HA	1:B:154:TYR:CD1	2.34	0.63
1:B:195:GLU:HG3	4:B:9654:HOH:O	2.00	0.61
1:C:75:LEU:HB2	1:C:157:VAL:O	2.00	0.61
1:C:61:GLN:NE2	1:C:63:ASN:HD21	1.90	0.60
1:C:197:LEU:C	4:C:9816:HOH:O	2.42	0.57
1:C:29:HIS:HD2	4:C:9754:HOH:O	1.87	0.57
1:D:74:GLY:CA	1:D:76:HIS:CE1	2.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:HG2	4:A:9206:HOH:O	2.04	0.57
1:A:8:LYS:HD3	1:A:25:ASP:HB3	1.89	0.55
1:C:76:HIS:ND1	3:C:9003:TDX:H3'	2.23	0.54
1:C:175:GLU:OE2	1:D:32:ASN:ND2	2.41	0.54
4:A:9072:HOH:O	1:B:29:HIS:HE1	1.91	0.54
1:D:159:TYR:OH	1:D:181:GLU:OE2	2.17	0.53
1:B:65:SER:HB2	4:B:9628:HOH:O	2.09	0.52
1:B:151:LYS:N	1:B:152:PRO:CD	2.73	0.52
1:D:61:GLN:NE2	1:D:63:ASN:HD21	1.97	0.51
1:C:123:ARG:HH11	1:C:197:LEU:HD22	1.77	0.49
1:B:61:GLN:NE2	1:B:63:ASN:HD21	1.91	0.48
1:B:151:LYS:HA	1:B:154:TYR:CE1	2.49	0.47
1:B:196:ASP:O	1:B:197:LEU:HB2	2.15	0.47
1:A:61:GLN:NE2	1:A:63:ASN:HD21	2.00	0.47
1:A:18:ILE:HB	1:A:21:MET:HE3	1.96	0.47
1:B:75:LEU:HB2	1:B:157:VAL:O	2.15	0.46
1:A:151:LYS:HA	1:A:154:TYR:CD2	2.51	0.46
1:A:63:ASN:HD22	1:B:38:GLU:HA	1.81	0.45
1:D:176:VAL:CG2	1:D:181:GLU:HG2	2.47	0.45
1:C:151:LYS:N	1:C:152:PRO:CD	2.79	0.45
1:D:75:LEU:HB2	1:D:157:VAL:O	2.17	0.44
1:A:16:GLU:HG2	4:A:9082:HOH:O	2.17	0.44
1:B:117:LYS:HE3	4:B:9787:HOH:O	2.18	0.43
1:A:151:LYS:N	1:A:152:PRO:CD	2.81	0.43
1:B:24:PHE:HB2	1:B:118:SER:OG	2.18	0.43
1:A:75:LEU:HB2	1:A:157:VAL:O	2.19	0.43
1:C:46:LEU:HB2	1:C:47:PRO:HD3	2.01	0.42
1:C:38:GLU:HA	1:D:63:ASN:HD22	1.84	0.42
1:A:8:LYS:NZ	4:A:9141:HOH:O	2.42	0.42
1:B:74:GLY:HA2	1:B:76:HIS:CE1	2.55	0.41
1:C:24:PHE:HB2	1:C:118:SER:OG	2.21	0.41
1:C:180:ASP:HA	1:C:183:HIS:CD2	2.56	0.41
1:A:69:LYS:O	1:A:70:ASN:HB2	2.21	0.40
1:C:176:VAL:CG1	1:C:180:ASP:HB2	2.52	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:THR:OG1	4:A:9019:HOH:O[1_655]	1.30	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLU:OE1	4:B:9697:HOH:O[1_455]	1.74	0.46
4:B:9654:HOH:O	4:D:9102:HOH:O[1_545]	1.79	0.41
4:A:9035:HOH:O	4:C:9823:HOH:O[2_546]	2.03	0.17
1:B:2:THR:N	4:A:9212:HOH:O[1_655]	2.06	0.14
4:A:9035:HOH:O	4:C:9689:HOH:O[2_546]	2.13	0.07
4:A:9035:HOH:O	4:C:9717:HOH:O[2_546]	2.17	0.03
4:A:9185:HOH:O	4:C:9715:HOH:O[2_546]	2.17	0.03

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	194/197 (98%)	189 (97%)	4 (2%)	1 (0%)	34	17
1	B	194/197 (98%)	190 (98%)	2 (1%)	2 (1%)	19	5
1	C	192/197 (98%)	185 (96%)	7 (4%)	0	100	100
1	D	192/197 (98%)	183 (95%)	9 (5%)	0	100	100
All	All	772/788 (98%)	747 (97%)	22 (3%)	3 (0%)	39	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	171	LEU
1	A	75	LEU
1	B	75	LEU

5.3.2 Protein sidechains (i)

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	168/169 (99%)	163 (97%)	5 (3%)	48	31
1	B	168/169 (99%)	156 (93%)	12 (7%)	18	6
1	C	166/169 (98%)	161 (97%)	5 (3%)	48	31
1	D	166/169 (98%)	158 (95%)	8 (5%)	31	14
All	All	668/676 (99%)	638 (96%)	30 (4%)	34	16

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	91	LYS
1	A	103	GLU
1	A	148	LEU
1	A	151	LYS
1	B	16	GLU
1	B	21	MET
1	B	41	GLN
1	B	91	LYS
1	B	123	ARG
1	B	146	TRP
1	B	148	LEU
1	B	157	VAL
1	B	167	LYS
1	B	170	ASN
1	B	171	LEU
1	B	193	ARG
1	C	41	GLN
1	C	91	LYS
1	C	148	LEU
1	C	167	LYS
1	C	196	ASP
1	D	16	GLU
1	D	41	GLN
1	D	91	LYS
1	D	148	LEU
1	D	149	GLU
1	D	150	LEU
1	D	163	SER
1	D	197	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	63	ASN
1	B	29	HIS
1	B	62	ASN
1	B	63	ASN
1	B	170	ASN
1	C	29	HIS
1	C	63	ASN
1	D	29	HIS
1	D	63	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)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	#$|Z| > 2$
3	TDX	A	9002	-	28,36,36	0.53	0	41,55,55	1.90	3 (7%)
3	TDX	B	9001	-	28,36,36	0.59	0	41,55,55	2.23	5 (12%)

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Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z \rvert > 2$	Counts	RMSZ	$\#\lvert Z \rvert > 2$
3	TDX	C	9003	-	28,36,36	0.58	0	41,55,55	2.16	4 (9%)
3	TDX	D	9004	-	28,36,36	0.65	0	41,55,55	2.22	5 (12%)

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	TDX	A	9002	-	-	0/17/50/50	0/3/3/3
3	TDX	B	9001	-	-	0/17/50/50	0/3/3/3
3	TDX	C	9003	-	-	0/17/50/50	0/3/3/3
3	TDX	D	9004	-	-	0/17/50/50	0/3/3/3

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	9004	TDX	C5-C4-N3	-7.46	116.83	125.14
3	B	9001	TDX	C5-C4-N3	-7.13	117.20	125.14
3	C	9003	TDX	C5-C4-N3	-7.10	117.23	125.14
3	A	9002	TDX	C5-C4-N3	-6.90	117.45	125.14
3	B	9001	TDX	O3'-C3'-C2'	-2.99	103.60	110.34
3	D	9004	TDX	O4B-C1B-N1	-2.78	102.90	107.72
3	C	9003	TDX	O3A-PA-O5B	-2.61	96.00	102.94
3	B	9001	TDX	O5'-C1'-O1'	-2.21	108.45	111.36
3	A	9002	TDX	C5M-C5-C4	2.15	122.83	120.05
3	C	9003	TDX	O2B-PB-O1B	2.15	124.19	112.53
3	D	9004	TDX	C2B-C1B-N1	2.50	120.23	114.16
3	D	9004	TDX	C5'-C4'-C3'	2.84	112.90	109.54
3	B	9001	TDX	O3'-C3'-C4'	6.05	120.93	110.00
3	A	9002	TDX	C4-N3-C2	7.80	121.99	115.25
3	B	9001	TDX	C4-N3-C2	8.19	122.33	115.25
3	C	9003	TDX	C4-N3-C2	9.23	123.22	115.25
3	D	9004	TDX	C4-N3-C2	9.67	123.60	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	9003	TDX	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, 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	196/197 (99%)	-0.10	2 (1%)	84 82	12, 17, 25, 38	0
1	B	196/197 (99%)	0.28	14 (7%)	19 15	15, 18, 27, 38	0
1	C	194/197 (98%)	-0.07	2 (1%)	84 82	14, 18, 26, 38	0
1	D	194/197 (98%)	-0.12	2 (1%)	84 82	15, 18, 27, 37	0
All	All	780/788 (98%)	-0.00	20 (2%)	59 54	12, 18, 27, 38	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	LEU	6.1
1	B	146	TRP	3.8
1	B	197	LEU	3.7
1	C	197	LEU	3.7
1	B	172	GLU	3.6
1	B	152	PRO	3.4
1	B	171	LEU	3.1
1	B	149	GLU	3.0
1	D	195	GLU	2.7
1	B	196	ASP	2.7
1	B	179	ALA	2.7
1	B	173	GLU	2.5
1	B	147	ALA	2.5
1	A	197	LEU	2.4
1	B	170	ASN	2.3
1	A	13	ARG	2.3
1	B	178	GLU	2.2
1	B	195	GLU	2.2
1	D	16	GLU	2.1
1	C	196	ASP	2.1

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	TDX	B	9001	34/34	0.77	0.21	2.38	41,64,67,68	1
3	TDX	A	9002	34/34	0.96	0.11	0.56	20,22,24,25	0
3	TDX	C	9003	34/34	0.96	0.10	0.18	19,23,27,27	0
3	TDX	D	9004	34/34	0.96	0.10	0.03	20,23,26,27	0
2	NI	C	9602	1/1	0.99	0.11	-	49,49,49,49	0
2	NI	B	9603	1/1	0.89	0.34	-	128,128,128,128	0

6.5 Other polymers (i)

There are no such residues in this entry.