



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 12, 2016 – 08:25 PM EDT

PDB ID : 5ESD
Title : Crystal Structure of M. tuberculosis MenD bound to ThDP and Mn²⁺
Authors : Johnston, J.M.; Jirgis, E.N.M.; Bashiri, G.; Bulloch, E.M.M.; Baker, E.N.
Deposited on : 2015-11-16
Resolution : 2.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027790

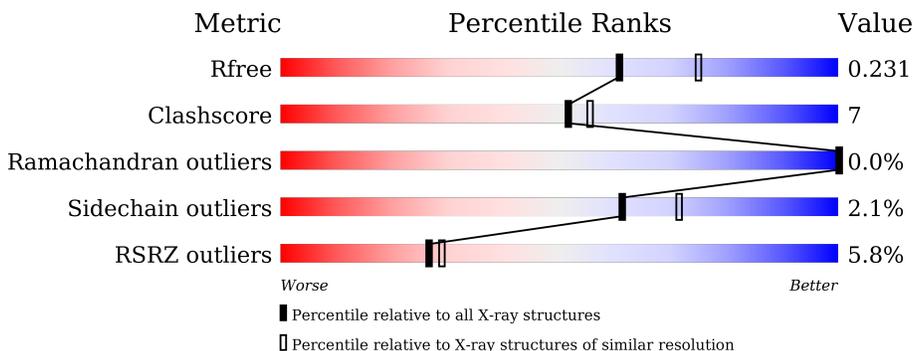
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	574	 5% 81% 13% 6%
1	B	574	 4% 80% 12% 7%
1	C	574	 6% 76% 18% 6%
1	D	574	 7% 79% 13% 6%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 16446 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 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	539	Total 3968	C 2476	N 737	O 743	S 12	0	2	0
1	B	532	Total 3934	C 2454	N 737	O 732	S 11	0	3	0
1	C	540	Total 3976	C 2478	N 740	O 748	S 10	0	1	0
1	D	541	Total 3979	C 2480	N 741	O 748	S 10	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P9WK11
A	-18	GLY	-	expression tag	UNP P9WK11
A	-17	SER	-	expression tag	UNP P9WK11
A	-16	SER	-	expression tag	UNP P9WK11
A	-15	HIS	-	expression tag	UNP P9WK11
A	-14	HIS	-	expression tag	UNP P9WK11
A	-13	HIS	-	expression tag	UNP P9WK11
A	-12	HIS	-	expression tag	UNP P9WK11
A	-11	HIS	-	expression tag	UNP P9WK11
A	-10	HIS	-	expression tag	UNP P9WK11
A	-9	SER	-	expression tag	UNP P9WK11
A	-8	SER	-	expression tag	UNP P9WK11
A	-7	GLY	-	expression tag	UNP P9WK11
A	-6	LEU	-	expression tag	UNP P9WK11
A	-5	VAL	-	expression tag	UNP P9WK11
A	-4	PRO	-	expression tag	UNP P9WK11
A	-3	ARG	-	expression tag	UNP P9WK11
A	-2	GLY	-	expression tag	UNP P9WK11
A	-1	SER	-	expression tag	UNP P9WK11
A	0	HIS	-	expression tag	UNP P9WK11

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP P9WK11
B	-18	GLY	-	expression tag	UNP P9WK11
B	-17	SER	-	expression tag	UNP P9WK11
B	-16	SER	-	expression tag	UNP P9WK11
B	-15	HIS	-	expression tag	UNP P9WK11
B	-14	HIS	-	expression tag	UNP P9WK11
B	-13	HIS	-	expression tag	UNP P9WK11
B	-12	HIS	-	expression tag	UNP P9WK11
B	-11	HIS	-	expression tag	UNP P9WK11
B	-10	HIS	-	expression tag	UNP P9WK11
B	-9	SER	-	expression tag	UNP P9WK11
B	-8	SER	-	expression tag	UNP P9WK11
B	-7	GLY	-	expression tag	UNP P9WK11
B	-6	LEU	-	expression tag	UNP P9WK11
B	-5	VAL	-	expression tag	UNP P9WK11
B	-4	PRO	-	expression tag	UNP P9WK11
B	-3	ARG	-	expression tag	UNP P9WK11
B	-2	GLY	-	expression tag	UNP P9WK11
B	-1	SER	-	expression tag	UNP P9WK11
B	0	HIS	-	expression tag	UNP P9WK11
C	-19	MET	-	initiating methionine	UNP P9WK11
C	-18	GLY	-	expression tag	UNP P9WK11
C	-17	SER	-	expression tag	UNP P9WK11
C	-16	SER	-	expression tag	UNP P9WK11
C	-15	HIS	-	expression tag	UNP P9WK11
C	-14	HIS	-	expression tag	UNP P9WK11
C	-13	HIS	-	expression tag	UNP P9WK11
C	-12	HIS	-	expression tag	UNP P9WK11
C	-11	HIS	-	expression tag	UNP P9WK11
C	-10	HIS	-	expression tag	UNP P9WK11
C	-9	SER	-	expression tag	UNP P9WK11
C	-8	SER	-	expression tag	UNP P9WK11
C	-7	GLY	-	expression tag	UNP P9WK11
C	-6	LEU	-	expression tag	UNP P9WK11
C	-5	VAL	-	expression tag	UNP P9WK11
C	-4	PRO	-	expression tag	UNP P9WK11
C	-3	ARG	-	expression tag	UNP P9WK11
C	-2	GLY	-	expression tag	UNP P9WK11
C	-1	SER	-	expression tag	UNP P9WK11
C	0	HIS	-	expression tag	UNP P9WK11
D	-19	MET	-	initiating methionine	UNP P9WK11
D	-18	GLY	-	expression tag	UNP P9WK11

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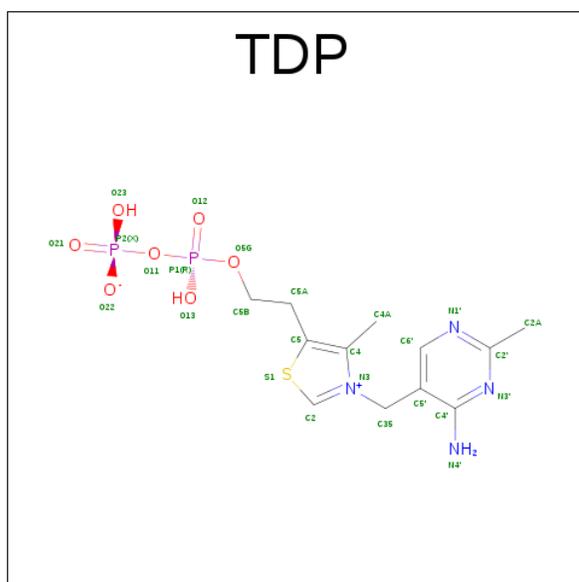
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	expression tag	UNP P9WK11
D	-16	SER	-	expression tag	UNP P9WK11
D	-15	HIS	-	expression tag	UNP P9WK11
D	-14	HIS	-	expression tag	UNP P9WK11
D	-13	HIS	-	expression tag	UNP P9WK11
D	-12	HIS	-	expression tag	UNP P9WK11
D	-11	HIS	-	expression tag	UNP P9WK11
D	-10	HIS	-	expression tag	UNP P9WK11
D	-9	SER	-	expression tag	UNP P9WK11
D	-8	SER	-	expression tag	UNP P9WK11
D	-7	GLY	-	expression tag	UNP P9WK11
D	-6	LEU	-	expression tag	UNP P9WK11
D	-5	VAL	-	expression tag	UNP P9WK11
D	-4	PRO	-	expression tag	UNP P9WK11
D	-3	ARG	-	expression tag	UNP P9WK11
D	-2	GLY	-	expression tag	UNP P9WK11
D	-1	SER	-	expression tag	UNP P9WK11
D	0	HIS	-	expression tag	UNP P9WK11

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0

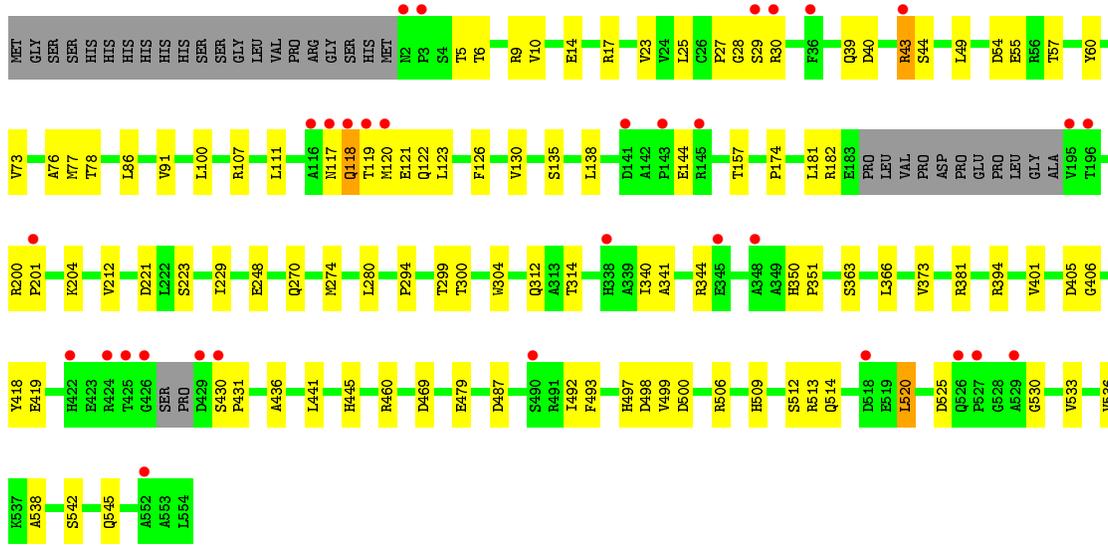
- Molecule 3 is THIAMIN DIPHOSPHATE (three-letter code: TDP) (formula: C₁₂H₁₈N₄O₇P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
3	A	1	Total 26	12	4	7	2	1	0	0
3	B	1	Total 26	12	4	7	2	1	0	0
3	C	1	Total 26	12	4	7	2	1	0	0
3	D	1	Total 26	12	4	7	2	1	0	0

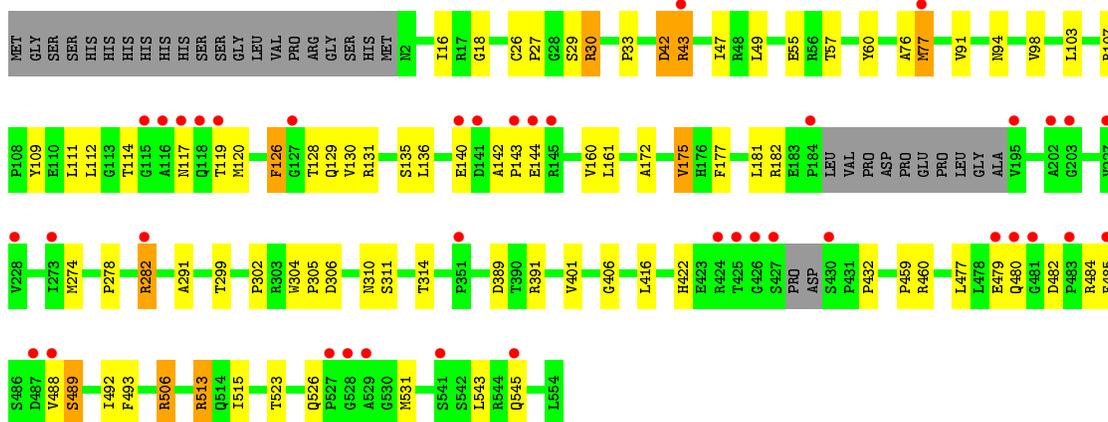
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	124	Total 124	O 124	0	0
4	B	125	Total 125	O 125	0	0
4	C	104	Total 104	O 104	0	0
4	D	128	Total 128	O 128	0	0



- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

Chain D: 7% 79% 13% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.62Å 138.66Å 165.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 2.25 19.81 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.81-2.25) 100.0 (19.81-2.25)	Depositor EDS
R_{merge}	0.43	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.26Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.210 , 0.235 0.202 , 0.231	Depositor DCC
R_{free} test set	5421 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	38.7	Xtrriage
Anisotropy	0.241	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16446	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TDP, MN

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	0.33	0/4056	0.50	0/5553
1	B	0.30	0/4020	0.50	0/5501
1	C	0.31	1/4059 (0.0%)	0.51	0/5555
1	D	0.32	0/4060	0.54	3/5556 (0.1%)
All	All	0.32	1/16195 (0.0%)	0.51	3/22165 (0.0%)

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	C	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	525	ASP	C-N	-5.04	1.22	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	282	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	D	42	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	506	ARG	NE-CZ-NH1	5.18	122.89	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	118	GLN	Peptide
1	D	77	MET	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	3968	0	4013	49	0
1	B	3934	0	3989	50	0
1	C	3976	0	4004	84	0
1	D	3979	0	4010	61	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	26	0	16	2	0
3	B	26	0	16	4	0
3	C	26	0	16	1	0
3	D	26	0	16	1	0
4	A	124	0	0	1	0
4	B	125	0	0	0	0
4	C	104	0	0	2	0
4	D	128	0	0	2	0
All	All	16446	0	16080	218	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 7.

The worst 5 of 218 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)
3:B:601:TDP:H2	3:B:601:TDP:C2	0.97	1.48
3:A:602:TDP:H2	3:A:602:TDP:C2	0.97	1.48
3:D:601:TDP:H2	3:D:601:TDP:C2	0.97	1.48
3:C:601:TDP:C2	3:C:601:TDP:H2	0.97	1.47
1:C:182:ARG:HH21	1:D:140:GLU:HG3	1.36	0.89

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	535/574 (93%)	529 (99%)	6 (1%)	0	100	100
1	B	527/574 (92%)	517 (98%)	10 (2%)	0	100	100
1	C	535/574 (93%)	518 (97%)	16 (3%)	1 (0%)	52	61
1	D	535/574 (93%)	518 (97%)	17 (3%)	0	100	100
All	All	2132/2296 (93%)	2082 (98%)	49 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	351	PRO

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	418/445 (94%)	413 (99%)	5 (1%)	78	87
1	B	413/445 (93%)	400 (97%)	13 (3%)	47	58
1	C	416/445 (94%)	409 (98%)	7 (2%)	68	79
1	D	417/445 (94%)	405 (97%)	12 (3%)	50	60
All	All	1664/1780 (94%)	1627 (98%)	37 (2%)	61	70

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	513[B]	ARG
1	C	73	VAL
1	D	506	ARG
1	B	551	LYS
1	C	43	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	31	ASN
1	D	545	GLN
1	D	350	HIS
1	C	39	GLN
1	D	526	GLN

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 8 ligands modelled in this entry, 4 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	TDP	A	602	2	21,27,27	1.74	2 (9%)	30,40,40	2.47	8 (26%)
3	TDP	B	601	2	21,27,27	1.33	2 (9%)	30,40,40	2.06	9 (30%)
3	TDP	C	601	2	21,27,27	1.34	2 (9%)	30,40,40	1.71	8 (26%)
3	TDP	D	601	2	21,27,27	1.41	2 (9%)	30,40,40	1.78	7 (23%)

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	TDP	A	602	2	-	0/16/17/17	0/2/2/2
3	TDP	B	601	2	-	0/16/17/17	0/2/2/2
3	TDP	C	601	2	-	0/16/17/17	0/2/2/2
3	TDP	D	601	2	-	0/16/17/17	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	TDP	C4-N3	-6.75	1.33	1.39
3	D	601	TDP	C4-N3	-4.76	1.35	1.39
3	B	601	TDP	C4-N3	-4.67	1.35	1.39
3	C	601	TDP	C4-N3	-4.52	1.35	1.39
3	B	601	TDP	C5'-C4'	2.59	1.47	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	TDP	C5'-C35-N3	-9.93	95.95	113.37
3	B	601	TDP	C5'-C4'-N4'	-3.65	116.87	122.27
3	D	601	TDP	C5A-C5-S1	-3.02	116.01	120.24
3	B	601	TDP	C5A-C5-S1	-2.97	116.08	120.24
3	A	602	TDP	C5'-C6'-N1'	-2.84	118.91	123.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	TDP	2	0
3	B	601	TDP	4	0
3	C	601	TDP	1	0
3	D	601	TDP	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	539/574 (93%)	0.11	31 (5%) 26 29	22, 35, 60, 80	0
1	B	532/574 (92%)	-0.00	23 (4%) 39 43	23, 35, 59, 76	0
1	C	540/574 (94%)	0.19	32 (5%) 26 28	24, 38, 65, 84	0
1	D	541/574 (94%)	0.14	39 (7%) 18 20	24, 35, 65, 86	0
All	All	2152/2296 (93%)	0.11	125 (5%) 26 29	22, 35, 62, 86	0

The worst 5 of 125 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	428	PRO	6.5
1	A	478	LEU	6.1
1	D	426	GLY	5.6
1	C	529	ALA	5.5
1	A	426	GLY	5.5

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(\AA^2)	Q<0.9
3	TDP	B	601	26/26	0.94	0.18	0.49	31,50,64,68	0
3	TDP	A	602	26/26	0.94	0.18	0.30	31,57,72,72	0
3	TDP	C	601	26/26	0.96	0.09	-1.02	31,34,39,40	0
3	TDP	D	601	26/26	0.98	0.09	-1.20	27,31,34,34	0
2	MN	A	601	1/1	0.99	0.07	-1.71	34,34,34,34	0
2	MN	B	602	1/1	0.98	0.05	-1.89	34,34,34,34	0
2	MN	C	602	1/1	0.99	0.02	-3.86	35,35,35,35	0
2	MN	D	602	1/1	1.00	0.04	-4.63	29,29,29,29	0

6.5 Other polymers

There are no such residues in this entry.