



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:00 PM GMT

PDB ID : 1N2S
Title : CRYSTAL STRUCTURE OF DTDP-6-DEOXY-L-LYXO-4-HEXULOSE
REDUCTASE (RMLD) IN COMPLEX WITH NADH
Authors : Blankenfeldt, W.; Kerr, I.D.; Giraud, M.F.; McMiken, H.J.; Leonard, G.A.;
Whitfield, C.; Messner, P.; Graninger, M.; Naismith, J.H.
Deposited on : 2002-10-24
Resolution : 2.00 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 (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

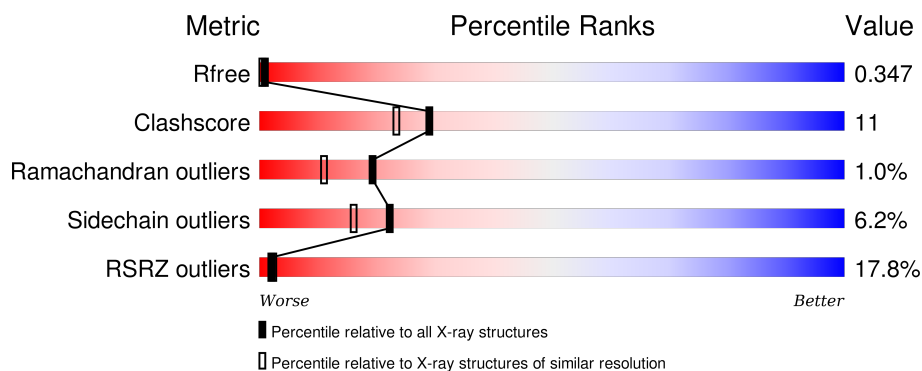
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	299	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2503 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.

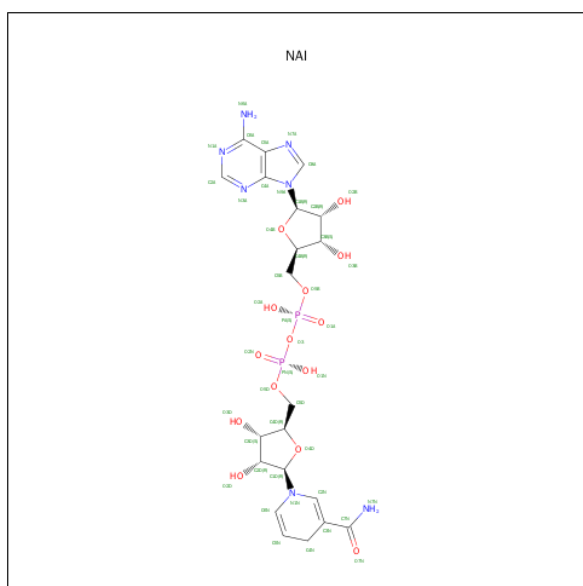
- Molecule 1 is a protein called dTDP-glucose oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2287	1451	396	433	7			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

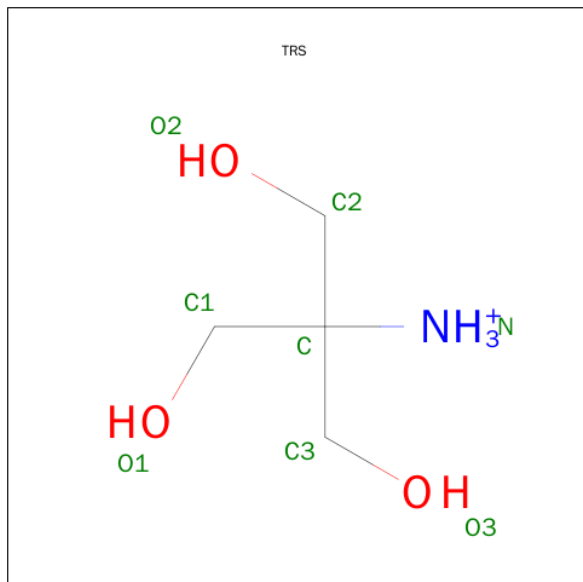
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



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

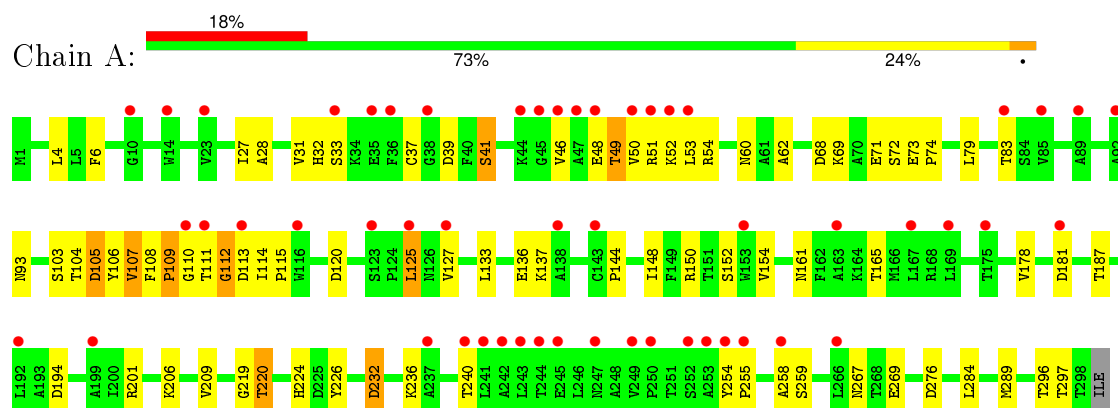
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	163	Total	O	0	0
			163	163		

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 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-glucose oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	47.44Å 71.57Å 82.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.70 – 2.00 54.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (81.70-2.00) 99.7 (54.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.199 , 0.253 0.310 , 0.347	Depositor DCC
R_{free} test set	996 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 19524 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2503	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% 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, 0.375 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: TRS, NAI, MG

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	0.95	2/2338 (0.1%)	1.02	9/3187 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	ALA	CA-CB	5.61	1.64	1.52
1	A	201	ARG	NE-CZ	-5.39	1.26	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	A	120	ASP	CB-CG-OD2	7.86	125.38	118.30
1	A	105	ASP	CB-CG-OD2	7.05	124.65	118.30
1	A	276	ASP	CB-CG-OD2	6.97	124.57	118.30
1	A	232	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	68	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	201	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	A	194	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	181	ASP	CB-CG-OD2	5.18	122.96	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	2287	0	2278	53	0
2	A	1	0	0	0	0
3	A	44	0	26	0	0
4	A	8	0	12	0	0
5	A	163	0	0	4	0
All	All	2503	0	2316	53	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 11.

All (53) 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:A:52:LYS:HB2	5:A:1032:HOH:O	1.77	0.84
1:A:133:LEU:HG	1:A:137:LYS:HZ2	1.47	0.77
1:A:103:SER:HB3	1:A:150:ARG:HG2	1.72	0.72
1:A:46:VAL:HA	1:A:49:THR:OG1	1.93	0.69
1:A:136:GLU:OE1	1:A:150:ARG:NH2	2.25	0.69
1:A:52:LYS:CB	5:A:1032:HOH:O	2.40	0.64
1:A:31:VAL:HG23	1:A:32:HIS:CD2	2.32	0.64
1:A:136:GLU:HB2	1:A:148:ILE:HD13	1.81	0.63
1:A:161:ASN:O	1:A:165:THR:HG23	2.00	0.61
1:A:109:PRO:HA	1:A:125:LEU:HG	1.82	0.60
1:A:267:ASN:OD1	1:A:269:GLU:HG2	2.02	0.59
1:A:27:ILE:CD1	1:A:53:LEU:HD22	2.32	0.59
1:A:105:ASP:C	1:A:107:VAL:H	2.04	0.58
1:A:110:GLY:O	1:A:111:THR:OG1	2.20	0.58
1:A:37:CYS:O	1:A:49:THR:HG21	2.06	0.56
1:A:54:ARG:HH11	1:A:54:ARG:HG3	1.71	0.55
1:A:111:THR:O	1:A:112:GLY:O	2.25	0.55
1:A:46:VAL:O	1:A:50:VAL:HG23	2.06	0.55
1:A:71:GLU:CG	1:A:258:ALA:HB2	2.38	0.53
1:A:27:ILE:HD13	1:A:53:LEU:HD22	1.89	0.53
1:A:54:ARG:HB2	5:A:1008:HOH:O	2.10	0.52
1:A:71:GLU:OE2	1:A:127:VAL:HG23	2.11	0.51
1:A:108:PHE:HB3	1:A:109:PRO:HD2	1.93	0.50
1:A:54:ARG:NH1	1:A:54:ARG:HG3	2.26	0.50
1:A:39:ASP:OD1	1:A:41:SER:HB2	2.12	0.49
1:A:71:GLU:HG2	1:A:258:ALA:HB2	1.94	0.49
1:A:73:GLU:O	1:A:73:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ASP:OD1	1:A:232:ASP:C	2.52	0.47
1:A:178:VAL:HG13	1:A:224:HIS:HB2	1.97	0.47
1:A:93:ASN:ND2	1:A:144:PRO:HD2	2.29	0.47
1:A:107:VAL:HG22	1:A:133:LEU:HD13	1.96	0.46
1:A:114:ILE:HA	1:A:115:PRO:HD3	1.81	0.46
1:A:112:GLY:O	1:A:113:ASP:HB2	2.16	0.46
1:A:254:TYR:HA	1:A:255:PRO:HD3	1.78	0.46
1:A:206:LYS:NZ	5:A:939:HOH:O	2.48	0.45
1:A:105:ASP:C	1:A:107:VAL:N	2.70	0.45
1:A:32:HIS:O	1:A:33:SER:C	2.55	0.45
1:A:53:LEU:O	1:A:54:ARG:HB2	2.17	0.44
1:A:105:ASP:O	1:A:107:VAL:N	2.50	0.44
1:A:107:VAL:CG2	1:A:133:LEU:HD13	2.48	0.44
1:A:154:VAL:HA	1:A:187:THR:O	2.18	0.43
1:A:114:ILE:O	1:A:114:ILE:HG22	2.18	0.43
1:A:4:LEU:HD21	1:A:6:PHE:CZ	2.55	0.42
1:A:73:GLU:N	1:A:74:PRO:HD3	2.35	0.42
1:A:60:ASN:ND2	1:A:62:ALA:H	2.16	0.42
1:A:69:LYS:HD2	1:A:69:LYS:HA	1.86	0.42
1:A:48:GLU:HA	1:A:51:ARG:CZ	2.50	0.41
1:A:206:LYS:O	1:A:209:VAL:HG22	2.21	0.41
1:A:31:VAL:HG23	1:A:32:HIS:CG	2.56	0.41
1:A:133:LEU:HG	1:A:137:LYS:NZ	2.28	0.40
1:A:232:ASP:OD1	1:A:236:LYS:HD2	2.21	0.40
1:A:79:LEU:HA	1:A:83:THR:HB	2.04	0.40
1:A:219:GLY:C	1:A:220:THR:HG22	2.41	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	296/299 (99%)	285 (96%)	8 (3%)	3 (1%)	19 11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLY
1	A	106	TYR
1	A	109	PRO

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	240/241 (100%)	225 (94%)	15 (6%)	22 16

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	SER
1	A	49	THR
1	A	72	SER
1	A	104	THR
1	A	107	VAL
1	A	125	LEU
1	A	152	SER
1	A	220	THR
1	A	226	TYR
1	A	240	THR
1	A	259	SER
1	A	284	LEU
1	A	289	MET
1	A	296	THR
1	A	297	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	60	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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$
4	TRS	A	601	-	7,7,7	1.06	1 (14%)	9,9,9	0.49	0
3	NAI	A	901	-	38,48,48	1.42	5 (13%)	48,73,73	2.35	15 (31%)

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
4	TRS	A	601	-	-	0/9/9/9	0/0/0/0
3	NAI	A	901	-	-	0/25/72/72	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	NAI	O3D-C3D	-2.84	1.36	1.43
4	A	601	TRS	C-N	-2.76	1.46	1.50
3	A	901	NAI	C2D-C3D	-2.52	1.46	1.53
3	A	901	NAI	PA-O2A	-2.30	1.45	1.54
3	A	901	NAI	O5D-C5D	-2.02	1.36	1.44
3	A	901	NAI	C2A-N3A	3.93	1.39	1.32

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	NAI	N3A-C2A-N1A	-8.96	122.03	128.89
3	A	901	NAI	C4B-O4B-C1B	-5.87	103.27	109.72
3	A	901	NAI	O3-PA-O5B	-4.27	91.60	102.94
3	A	901	NAI	C2B-C1B-N9A	-4.19	107.89	114.29
3	A	901	NAI	C4D-O4D-C1D	-2.98	102.96	109.52
3	A	901	NAI	PN-O3-PA	-2.52	125.65	132.73
3	A	901	NAI	C2B-C3B-C4B	-2.32	97.84	102.61
3	A	901	NAI	O3D-C3D-C4D	-2.26	104.27	111.05
3	A	901	NAI	C1B-N9A-C4A	-2.25	123.54	126.94
3	A	901	NAI	O1N-PN-O2N	2.24	124.64	112.53
3	A	901	NAI	O4B-C4B-C3B	2.44	110.05	105.15
3	A	901	NAI	O7N-C7N-N7N	2.47	128.91	122.76
3	A	901	NAI	O2D-C2D-C1D	3.01	120.45	109.94
3	A	901	NAI	O4B-C1B-N9A	3.06	114.50	108.10
3	A	901	NAI	O4D-C4D-C3D	3.65	112.50	105.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	298/299 (99%)	1.36	53 (17%) 2 2	22, 30, 40, 59	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	ALA	9.6
1	A	254	TYR	7.0
1	A	47	ALA	6.0
1	A	252	SER	5.5
1	A	113	ASP	5.3
1	A	45	GLY	5.0
1	A	241	LEU	4.4
1	A	48	GLU	4.1
1	A	245	GLU	3.9
1	A	242	ALA	3.8
1	A	116	TRP	3.8
1	A	255	PRO	3.7
1	A	123	SER	3.6
1	A	243	LEU	3.5
1	A	44	LYS	3.5
1	A	53	LEU	3.4
1	A	247	ASN	3.3
1	A	46	VAL	3.3
1	A	23	VAL	3.2
1	A	125	LEU	3.1
1	A	50	VAL	3.1
1	A	36	PHE	3.0
1	A	110	GLY	3.0
1	A	52	LYS	2.9
1	A	250	PRO	2.8
1	A	175	THR	2.8
1	A	244	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	167	LEU	2.7
1	A	169	LEU	2.7
1	A	92	ALA	2.7
1	A	266	LEU	2.7
1	A	258	ALA	2.6
1	A	240	THR	2.5
1	A	35	GLU	2.5
1	A	51	ARG	2.5
1	A	143	CYS	2.5
1	A	199	ALA	2.4
1	A	237	ALA	2.4
1	A	111	THR	2.4
1	A	85	VAL	2.3
1	A	127	VAL	2.3
1	A	192	LEU	2.3
1	A	33	SER	2.3
1	A	181	ASP	2.3
1	A	38	GLY	2.2
1	A	89	ALA	2.1
1	A	14	TRP	2.1
1	A	153	TRP	2.1
1	A	249	VAL	2.1
1	A	10	GLY	2.1
1	A	138	ALA	2.0
1	A	163	ALA	2.0
1	A	83	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(\AA^2)	Q<0.9
3	NAI	A	901	44/44	0.93	0.16	-0.56	26,32,36,37	0
2	MG	A	501	1/1	0.88	0.12	-	31,31,31,31	1
4	TRS	A	601	8/8	0.84	0.17	-	52,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.