



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2022 – 01:31 PM EDT

PDB ID : 4Q0V
Title : Crystal structure of Acinetobacter sp. DL28 L-ribose isomerase mutant E204Q
in complex with L-ribulose
Authors : Yoshida, H.; Yoshihara, A.; Teraoka, M.; Izumori, K.; Kamitori, S.
Deposited on : 2014-04-02
Resolution : 1.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.29
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) : 2.29

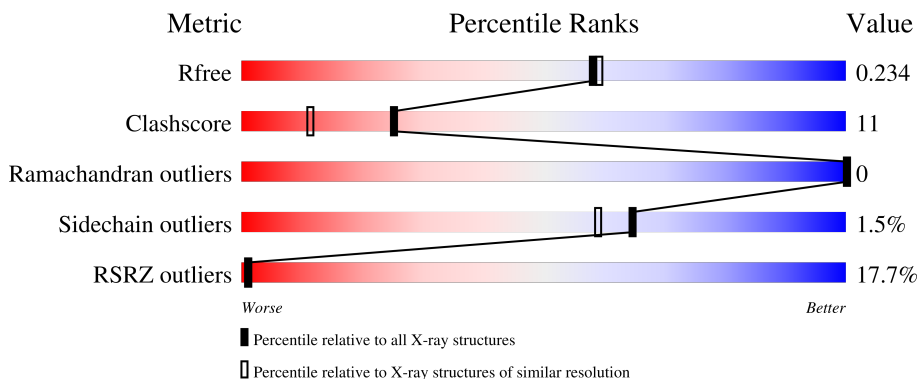
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 of 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	260	

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
4	RUU	A	503	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2109 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 L-Ribose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	249	1930	1220	332	367	11	0	0	0

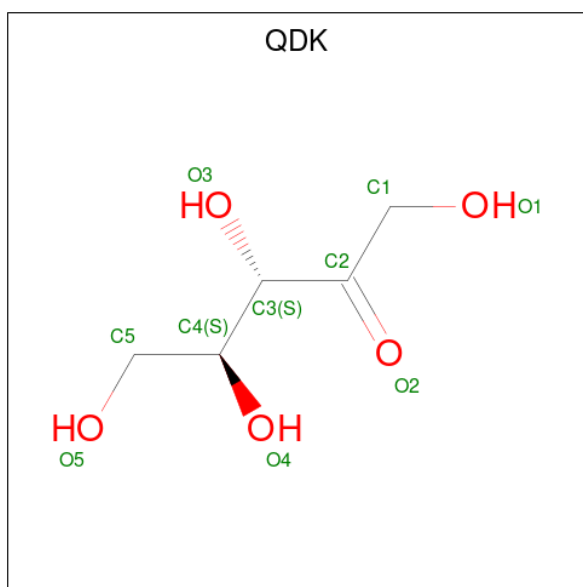
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP Q93UQ5
A	-9	ARG	-	expression tag	UNP Q93UQ5
A	-8	GLY	-	expression tag	UNP Q93UQ5
A	-7	SER	-	expression tag	UNP Q93UQ5
A	-6	HIS	-	expression tag	UNP Q93UQ5
A	-5	HIS	-	expression tag	UNP Q93UQ5
A	-4	HIS	-	expression tag	UNP Q93UQ5
A	-3	HIS	-	expression tag	UNP Q93UQ5
A	-2	HIS	-	expression tag	UNP Q93UQ5
A	-1	HIS	-	expression tag	UNP Q93UQ5
A	0	GLY	-	expression tag	UNP Q93UQ5
A	1	SER	-	expression tag	UNP Q93UQ5
A	2	ALA	-	expression tag	UNP Q93UQ5
A	204	GLN	GLU	engineered mutation	UNP Q93UQ5

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

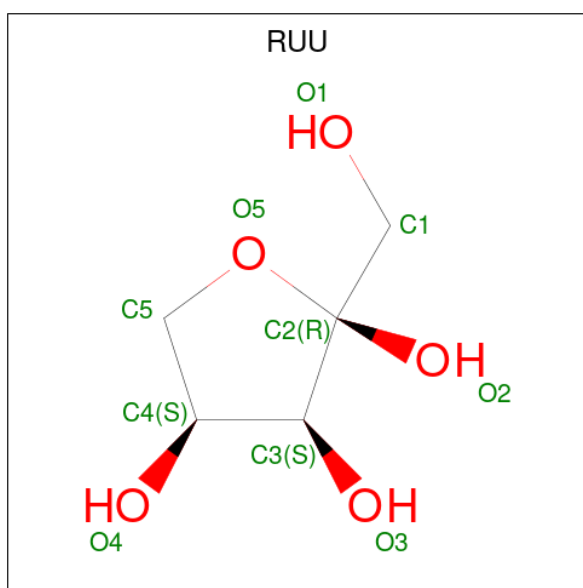
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Co	0	0
			1	1		

- Molecule 3 is L-ribulose (three-letter code: QDK) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is alpha-L-ribofuranose (three-letter code: RUU) (formula: $C_5H_{10}O_5$).



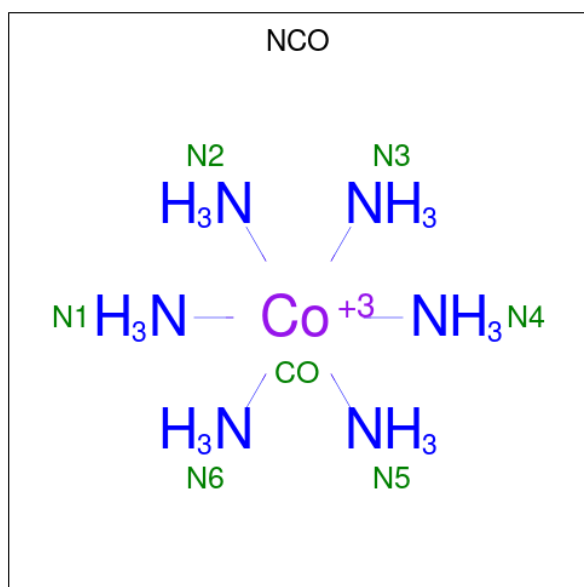
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		
4	A	1	Total	C	O	0	0
			10	5	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		
4	A	1	Total	C	O	0	0
			10	5	5		
4	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula: $\text{CoH}_{18}\text{N}_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Co	N	0	0
			7	1	6		

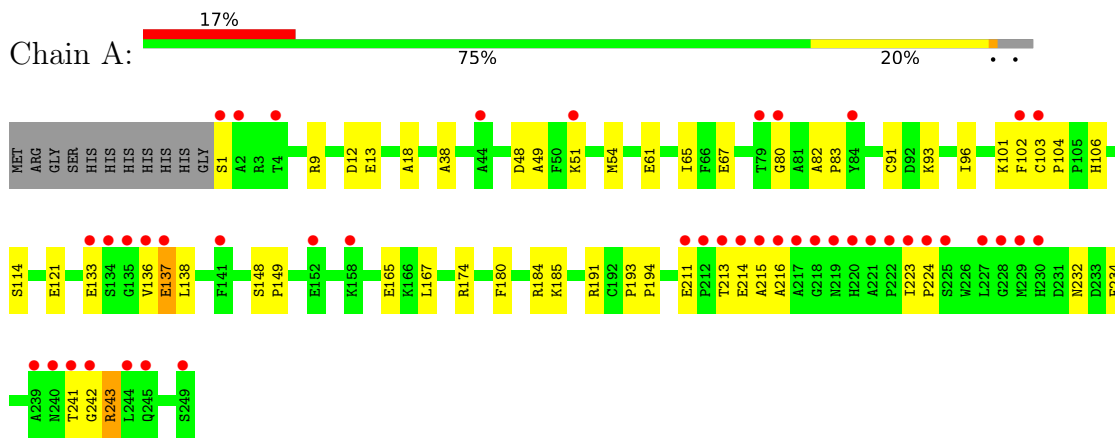
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	101	Total	O	0	0
			101	101		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: L-Ribose isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	95.85Å 107.35Å 118.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.77 – 1.98 21.77 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.8 (21.77-1.98) 100.0 (21.77-1.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 1.98Å)	Xtrriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.203 , 0.243 0.198 , 0.234	Depositor DCC
R_{free} test set	2122 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtrriage
Anisotropy	0.362	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2109	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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: CO, NCO, QDK, RUU

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	0/1988	0.61	1/2704 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	CYS	N-CA-C	-7.80	89.92	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1930	0	1847	42	0
2	A	1	0	0	0	0
3	A	20	0	19	0	0
4	A	50	0	50	10	0
5	A	7	0	0	0	0
6	A	101	0	0	0	0
All	All	2109	0	1916	42	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 (42) 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:215:ALA:HB3	4:A:503:RUU:H9	1.71	0.72
1:A:12:ASP:OD2	4:A:506:RUU:H1	1.91	0.70
1:A:91:CYS:SG	1:A:93:LYS:HD2	2.31	0.70
1:A:241:THR:HG23	1:A:242:GLY:H	1.57	0.69
1:A:211:GLU:HG2	1:A:232:ASN:HD21	1.62	0.63
1:A:67:GLU:H	4:A:503:RUU:C1	2.12	0.63
1:A:243:ARG:O	1:A:243:ARG:HD3	1.99	0.62
1:A:67:GLU:H	4:A:503:RUU:H2	1.66	0.60
1:A:49:ALA:HB1	1:A:54:MET:HE1	1.85	0.58
1:A:65:ILE:O	4:A:503:RUU:H1	2.05	0.57
1:A:241:THR:HG23	1:A:242:GLY:N	2.19	0.57
1:A:9:ARG:O	1:A:13:GLU:HG3	2.05	0.55
1:A:65:ILE:HG21	1:A:93:LYS:HE2	1.88	0.54
1:A:133:GLU:OE1	1:A:136:VAL:HG11	2.08	0.54
1:A:18:ALA:HB1	1:A:96:ILE:HD12	1.90	0.52
1:A:106:HIS:HB3	1:A:234:PHE:CD1	2.44	0.51
1:A:48:ASP:O	1:A:51:LYS:HB2	2.10	0.51
1:A:167:LEU:HD12	1:A:167:LEU:N	2.26	0.51
1:A:121:GLU:OE2	1:A:174:ARG:HD3	2.12	0.50
1:A:223:ILE:HG23	1:A:224:PRO:HD2	1.95	0.48
1:A:61:GLU:CD	1:A:104:PRO:HB3	2.35	0.47
1:A:114:SER:HA	1:A:180:PHE:O	2.13	0.47
1:A:165:GLU:HA	4:A:507:RUU:O4	2.15	0.47
1:A:133:GLU:HB3	1:A:136:VAL:CG1	2.45	0.47
1:A:38:ALA:HA	4:A:503:RUU:O2	2.15	0.46
1:A:133:GLU:HB3	1:A:136:VAL:HG13	1.98	0.45
1:A:211:GLU:HG2	1:A:232:ASN:ND2	2.29	0.45
1:A:137:GLU:OE1	1:A:138:LEU:N	2.49	0.44
1:A:193:PRO:HA	1:A:194:PRO:HD3	1.88	0.44
1:A:1:SER:O	1:A:51:LYS:HE3	2.17	0.44
1:A:82:ALA:N	1:A:83:PRO:HD2	2.32	0.44
1:A:102:PHE:CD2	1:A:191:ARG:HB3	2.53	0.44
1:A:148:SER:HB3	1:A:149:PRO:HD2	1.98	0.44
1:A:211:GLU:O	1:A:213:THR:N	2.48	0.43
1:A:9:ARG:HA	4:A:506:RUU:O3	2.19	0.43
1:A:54:MET:CE	1:A:101:LYS:HE2	2.49	0.42
1:A:243:ARG:HD3	1:A:243:ARG:C	2.40	0.42
1:A:213:THR:N	1:A:216:ALA:HB3	2.36	0.41
1:A:80:GLY:O	1:A:83:PRO:HD2	2.20	0.41
1:A:67:GLU:N	4:A:503:RUU:H2	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ALA:CB	4:A:503:RUU:H9	2.47	0.40
1:A:184:ARG:O	1:A:185:LYS:HB2	2.22	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	247/260 (95%)	236 (96%)	11 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	205/214 (96%)	202 (98%)	3 (2%)	65 59

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	GLU
1	A	214	GLU
1	A	243	ARG

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

Mol	Chain	Res	Type
1	A	204	GLN
1	A	219	ASN
1	A	220	HIS
1	A	232	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	RUU	A	508	-	9,10,10	0.54	0	8,15,15	1.32	1 (12%)
4	RUU	A	506	-	9,10,10	0.57	0	8,15,15	1.30	1 (12%)
5	NCO	A	509	-	6,6,6	4.49	6 (100%)	-	-	-
4	RUU	A	505	-	9,10,10	0.60	0	8,15,15	1.36	1 (12%)
4	RUU	A	503	-	9,10,10	0.53	0	8,15,15	1.18	1 (12%)
4	RUU	A	507	-	9,10,10	0.54	0	8,15,15	1.40	1 (12%)
3	QDK	A	504	-	7,9,9	0.49	0	5,11,11	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	QDK	A	502	2	7,9,9	0.52	0	5,11,11	0.73	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
4	RUU	A	508	-	-	1/3/19/19	0/1/1/1
4	RUU	A	506	-	-	1/3/19/19	0/1/1/1
4	RUU	A	505	-	-	1/3/19/19	0/1/1/1
4	RUU	A	503	-	-	3/3/19/19	0/1/1/1
4	RUU	A	507	-	-	1/3/19/19	0/1/1/1
3	QDK	A	504	-	-	6/12/12/12	-
3	QDK	A	502	2	-	2/12/12/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	509	NCO	CO-N5	-4.77	1.80	1.96
5	A	509	NCO	CO-N6	-4.51	1.81	1.96
5	A	509	NCO	CO-N1	-4.46	1.81	1.96
5	A	509	NCO	CO-N4	-4.41	1.81	1.96
5	A	509	NCO	CO-N2	-4.38	1.81	1.96
5	A	509	NCO	CO-N3	-4.38	1.81	1.96

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	507	RUU	C5-C4-C3	3.14	105.94	101.94
4	A	505	RUU	C5-C4-C3	3.05	105.83	101.94
4	A	508	RUU	C5-C4-C3	2.92	105.66	101.94
4	A	506	RUU	C5-C4-C3	2.88	105.60	101.94
4	A	503	RUU	C5-C4-C3	2.47	105.09	101.94

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	QDK	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	502	QDK	O2-C2-C3-O3
3	A	504	QDK	O1-C1-C2-O2
3	A	504	QDK	C1-C2-C3-O3
3	A	504	QDK	C1-C2-C3-C4
3	A	504	QDK	O2-C2-C3-O3
3	A	504	QDK	O2-C2-C3-C4
4	A	503	RUU	O1-C1-C2-C3
4	A	505	RUU	O1-C1-C2-C3
4	A	506	RUU	O1-C1-C2-C3
4	A	508	RUU	O1-C1-C2-C3
4	A	503	RUU	O1-C1-C2-O2
4	A	503	RUU	O1-C1-C2-O5
3	A	504	QDK	O1-C1-C2-C3
4	A	507	RUU	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	506	RUU	2	0
4	A	503	RUU	7	0
4	A	507	RUU	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

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	249/260 (95%)	1.16	44 (17%) 1 1	18, 27, 60, 79	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	GLY	10.8
1	A	219	ASN	9.7
1	A	217	ALA	9.6
1	A	1	SER	9.4
1	A	227	LEU	8.3
1	A	216	ALA	8.2
1	A	213	THR	8.1
1	A	220	HIS	8.0
1	A	212	PRO	7.1
1	A	2	ALA	7.1
1	A	228	GLY	6.9
1	A	214	GLU	6.1
1	A	134	SER	5.4
1	A	245	GLN	5.1
1	A	221	ALA	5.1
1	A	229	MET	5.0
1	A	135	GLY	4.6
1	A	240	ASN	4.5
1	A	244	LEU	4.5
1	A	230	HIS	4.3
1	A	136	VAL	3.8
1	A	158	LYS	3.6
1	A	225	SER	3.5
1	A	224	PRO	3.3
1	A	223	ILE	3.3
1	A	215	ALA	3.3
1	A	249	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	152	GLU	3.2
1	A	211	GLU	3.0
1	A	241	THR	3.0
1	A	79	THR	2.9
1	A	141	PHE	2.8
1	A	239	ALA	2.7
1	A	4	THR	2.7
1	A	103	CYS	2.6
1	A	84	TYR	2.5
1	A	222	PRO	2.5
1	A	137	GLU	2.4
1	A	133	GLU	2.3
1	A	242	GLY	2.3
1	A	51	LYS	2.2
1	A	102	PHE	2.2
1	A	44	ALA	2.1
1	A	80	GLY	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 monosaccharides 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	RUU	A	507	10/10	0.65	0.31	77,78,79,79	0
4	RUU	A	506	10/10	0.72	0.33	69,71,72,72	0
3	QDK	A	504	10/10	0.77	0.22	54,61,62,63	0
4	RUU	A	503	10/10	0.77	0.26	45,55,56,57	0
4	RUU	A	508	10/10	0.84	0.20	44,53,54,55	0
5	NCO	A	509	7/7	0.84	0.42	38,39,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	RUU	A	505	10/10	0.85	0.24	66,67,68,68	0
3	QDK	A	502	10/10	0.86	0.22	28,40,51,51	0
2	CO	A	501	1/1	0.99	0.03	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.