WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 26, 2023 – 06:07 PM EDT

PDB ID	:	3ITL
Title	:	Crystal structure of Pseudomonas stutzeri L-rhamnose isomerase mutant D327N in complex with L-rhamnulose
Authors	:	Yoshida, H.; Yamaji, M.; Ishii, T.; Izumori, K.; Kamitori, S.
Deposited on	:	2009-08-28
Resolution	:	1.70 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
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	:	2.36
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)	:	2.36

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 1.70 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.
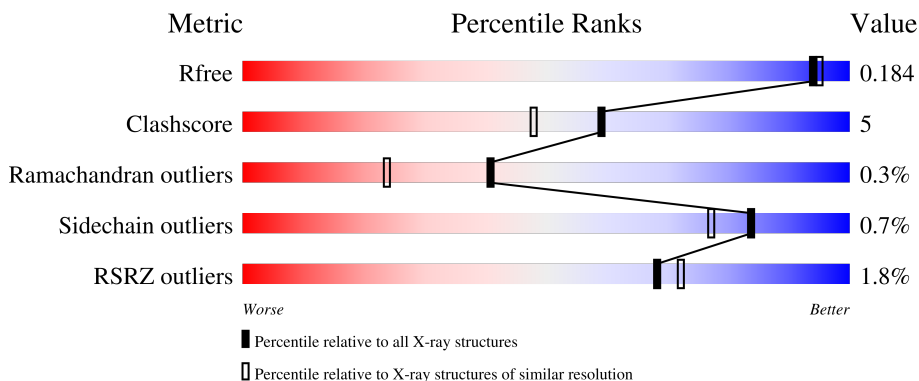
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	438	86% / 10% ·
1	B	438	2% / 84% / 12% ·
1	C	438	3% / 86% / 12% ·
1	D	438	87% / 9% ·

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 15023 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-rhamnose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3260	2048	585	618	9			
1	B	421	Total	C	N	O	S	0	0	0
			3260	2048	585	618	9			
1	C	428	Total	C	N	O	S	0	0	0
			3301	2073	592	627	9			
1	D	419	Total	C	N	O	S	0	0	0
			3251	2042	583	617	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	ASN	ASP	engineered mutation	UNP Q75WH8
A	327	ASN	ASP	engineered mutation	UNP Q75WH8
A	431	GLY	-	expression tag	UNP Q75WH8
A	432	SER	-	expression tag	UNP Q75WH8
A	433	HIS	-	expression tag	UNP Q75WH8
A	434	HIS	-	expression tag	UNP Q75WH8
A	435	HIS	-	expression tag	UNP Q75WH8
A	436	HIS	-	expression tag	UNP Q75WH8
A	437	HIS	-	expression tag	UNP Q75WH8
A	438	HIS	-	expression tag	UNP Q75WH8
B	150	ASN	ASP	engineered mutation	UNP Q75WH8
B	327	ASN	ASP	engineered mutation	UNP Q75WH8
B	431	GLY	-	expression tag	UNP Q75WH8
B	432	SER	-	expression tag	UNP Q75WH8
B	433	HIS	-	expression tag	UNP Q75WH8
B	434	HIS	-	expression tag	UNP Q75WH8
B	435	HIS	-	expression tag	UNP Q75WH8
B	436	HIS	-	expression tag	UNP Q75WH8
B	437	HIS	-	expression tag	UNP Q75WH8
B	438	HIS	-	expression tag	UNP Q75WH8
C	150	ASN	ASP	engineered mutation	UNP Q75WH8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	327	ASN	ASP	engineered mutation	UNP Q75WH8
C	431	GLY	-	expression tag	UNP Q75WH8
C	432	SER	-	expression tag	UNP Q75WH8
C	433	HIS	-	expression tag	UNP Q75WH8
C	434	HIS	-	expression tag	UNP Q75WH8
C	435	HIS	-	expression tag	UNP Q75WH8
C	436	HIS	-	expression tag	UNP Q75WH8
C	437	HIS	-	expression tag	UNP Q75WH8
C	438	HIS	-	expression tag	UNP Q75WH8
D	150	ASN	ASP	engineered mutation	UNP Q75WH8
D	327	ASN	ASP	engineered mutation	UNP Q75WH8
D	431	GLY	-	expression tag	UNP Q75WH8
D	432	SER	-	expression tag	UNP Q75WH8
D	433	HIS	-	expression tag	UNP Q75WH8
D	434	HIS	-	expression tag	UNP Q75WH8
D	435	HIS	-	expression tag	UNP Q75WH8
D	436	HIS	-	expression tag	UNP Q75WH8
D	437	HIS	-	expression tag	UNP Q75WH8
D	438	HIS	-	expression tag	UNP Q75WH8

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

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

- Molecule 3 is 6-deoxy-beta-L-fructofuranose (three-letter code: LRH) (formula: $C_6H_{12}O_5$).

LRH

O1

HO

O5

O

C6

C5(S)

C2(S)

C1

OH

O2

C4(R)

C3(R)

HO

OH

O4

O3
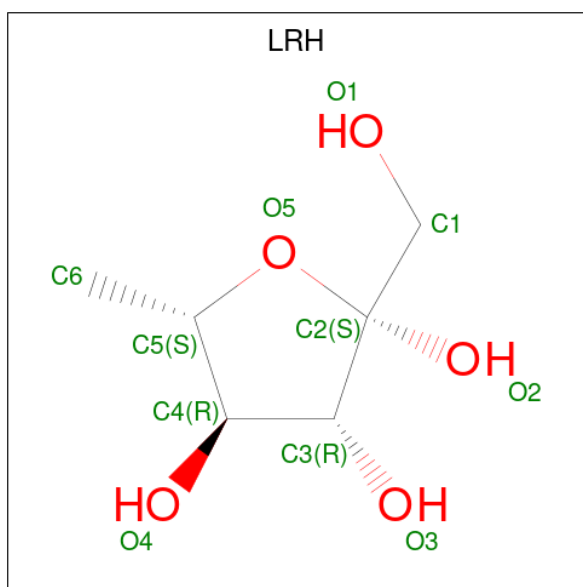
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 11	C 6	O 5	0	0
3	B	1	Total 11	C 6	O 5	0	0
3	C	1	Total 11	C 6	O 5	0	0
3	D	1	Total 11	C 6	O 5	0	0

- Molecule 4 is water.

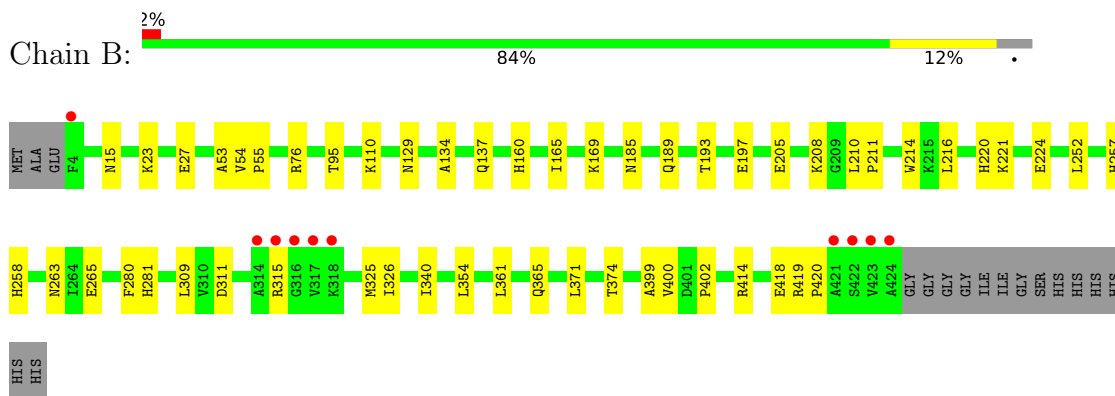| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	493	Total 493	O 493	0	0
4	B	490	Total 490	O 490	0	0
4	C	443	Total 443	O 443	0	0
4	D	473	Total 473	O 473	0	0

3 Residue-property plots ⓘ

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.
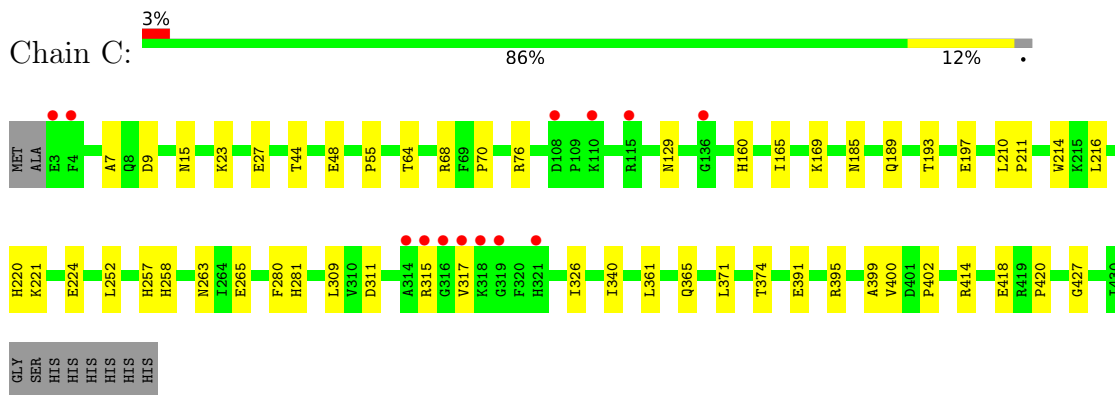
- Molecule 1: L-rhamnose isomerase
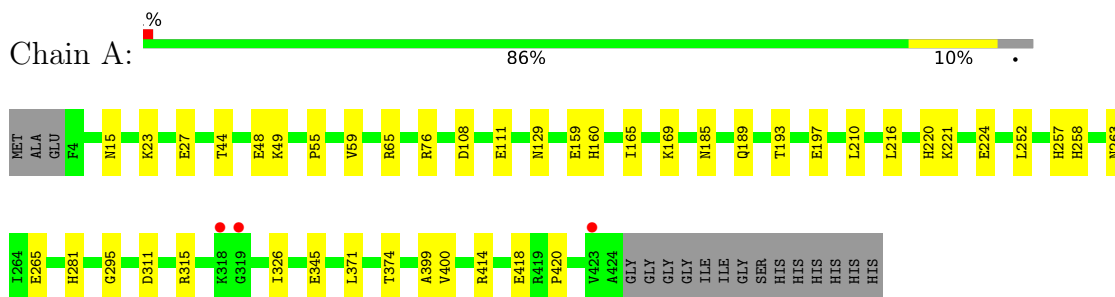
Chain A:

- Molecule 1: L-rhamnose isomerase

Chain B:

- Molecule 1: L-rhamnose isomerase

Chain C:

- Molecule 1: L-rhamnose isomerase

Chain D:

%

87% 9%

MET ALA E3 F4 Q8 R13 E14 N15 K23 E27 F66 A67 R76 D108 E111 N129 H160 N185 G188 Q189 T193 E197 H220 K221 E224 H257 H258 N263 I264 E265 L277 G295 F320 I340 E345 L361

Q365 E366 T374 R382 A399 V400 D401 P402 R414 E418 R419 P420 A421 SER VAL ALA GLY GLY GLY ILE ILE GLY SER HIS HIS HIS HIS HIS HIS
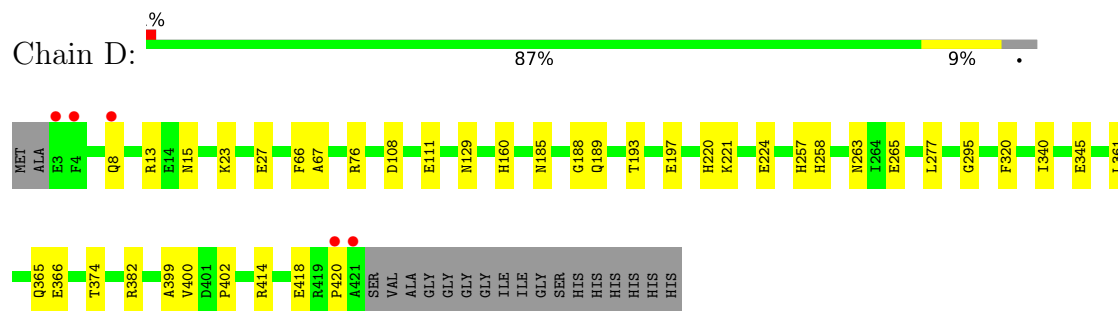
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.70Å 104.63Å 115.10Å 90.00° 108.14° 90.00°	Depositor
Resolution (Å)	42.12 – 1.70 42.12 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.2 (42.12-1.70) 96.2 (42.12-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.15 (at 1.70Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.165 , 0.188 0.160 , 0.184	Depositor DCC
R_{free} test set	17627 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å^2)	12.5	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 54.3	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15023	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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, 0.333 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: LRH, 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	0.30	0/3332	0.55	0/4518
1	B	0.30	0/3332	0.54	0/4518
1	C	0.28	0/3373	0.52	0/4572
1	D	0.29	0/3323	0.53	0/4505
All	All	0.29	0/13360	0.54	0/18113

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 (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	3260	0	3167	29	0
1	B	3260	0	3167	32	0
1	C	3301	0	3207	32	0
1	D	3251	0	3154	28	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	11	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	9	0	0
3	C	11	0	9	0	0
3	D	11	0	9	0	0
4	A	493	0	0	4	0
4	B	490	0	0	3	0
4	C	443	0	0	0	0
4	D	473	0	0	4	0
All	All	15023	0	12731	121	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 5.

The worst 5 of 121 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:129:ASN:H	1:A:160:HIS:HE1	1.18	0.88
1:B:129:ASN:H	1:B:160:HIS:HE1	1.24	0.84
1:C:129:ASN:H	1:C:160:HIS:HE1	1.27	0.82
1:A:129:ASN:H	1:A:160:HIS:CE1	1.98	0.81
1:D:129:ASN:H	1:D:160:HIS:HE1	1.24	0.80

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	419/438 (96%)	408 (97%)	10 (2%)	1 (0%)	47	30
1	B	419/438 (96%)	407 (97%)	11 (3%)	1 (0%)	47	30
1	C	426/438 (97%)	415 (97%)	9 (2%)	2 (0%)	29	13
1	D	417/438 (95%)	406 (97%)	10 (2%)	1 (0%)	47	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1681/1752 (96%)	1636 (97%)	40 (2%)	5 (0%)	41 24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	GLU
1	B	224	GLU
1	C	224	GLU
1	D	224	GLU
1	C	317	VAL

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	330/341 (97%)	327 (99%)	3 (1%)	78	70
1	B	330/341 (97%)	327 (99%)	3 (1%)	78	70
1	C	333/341 (98%)	331 (99%)	2 (1%)	86	80
1	D	329/341 (96%)	328 (100%)	1 (0%)	92	89
All	All	1322/1364 (97%)	1313 (99%)	9 (1%)	84	77

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	374	THR
1	D	374	THR
1	B	354	LEU
1	B	371	LEU
1	B	374	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	160	HIS
1	C	344	ASN
1	C	258	HIS
1	D	15	ASN
1	B	160	HIS

5.3.3   RNA   ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains   ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5   Carbohydrates   ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry   ⓘ

Of 12 ligands modelled in this entry, 8 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	LRH	B	602	2	10,11,11	0.44	0	10,17,17	1.18	1 (10%)
3	LRH	D	604	2	10,11,11	0.37	0	10,17,17	1.15	1 (10%)
3	LRH	A	601	2	10,11,11	0.42	0	10,17,17	1.16	1 (10%)
3	LRH	C	603	2	10,11,11	0.36	0	10,17,17	1.17	1 (10%)

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	LRH	B	602	2	-	1/3/22/22	0/1/1/1
3	LRH	D	604	2	-	1/3/22/22	0/1/1/1
3	LRH	A	601	2	-	1/3/22/22	0/1/1/1
3	LRH	C	603	2	-	1/3/22/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	603	LRH	O5-C5-C4	2.59	106.61	102.93
3	B	602	LRH	O5-C5-C4	2.58	106.60	102.93
3	D	604	LRH	O5-C5-C4	2.42	106.36	102.93
3	A	601	LRH	O5-C5-C4	2.28	106.17	102.93

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	LRH	O1-C1-C2-C3
3	B	602	LRH	O1-C1-C2-C3
3	C	603	LRH	O1-C1-C2-C3
3	D	604	LRH	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	A	421/438 (96%)	-0.34	3 (0%)	87	90	6, 11, 23, 35	0
1	B	421/438 (96%)	-0.13	10 (2%)	59	63	6, 13, 26, 49	0
1	C	428/438 (97%)	-0.00	13 (3%)	50	54	7, 15, 31, 56	0
1	D	419/438 (95%)	-0.19	5 (1%)	79	82	7, 12, 24, 48	0
All	All	1689/1752 (96%)	-0.16	31 (1%)	68	72	6, 13, 26, 56	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	319	GLY	11.1
1	B	423	VAL	6.0
1	C	317	VAL	5.9
1	B	4	PHE	5.8
1	D	4	PHE	5.6

6.2   Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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
3	LRH	B	602	11/11	0.87	0.12	12,15,17,17	0
3	LRH	C	603	11/11	0.89	0.10	14,16,17,18	0
3	LRH	A	601	11/11	0.94	0.09	7,9,10,14	0
3	LRH	D	604	11/11	0.94	0.09	10,11,14,14	0
2	MN	C	505	1/1	1.00	0.03	14,14,14,14	0
2	MN	C	506	1/1	1.00	0.03	11,11,11,11	0
2	MN	D	507	1/1	1.00	0.04	9,9,9,9	0
2	MN	D	508	1/1	1.00	0.05	8,8,8,8	0
2	MN	A	501	1/1	1.00	0.03	8,8,8,8	0
2	MN	A	502	1/1	1.00	0.05	7,7,7,7	0
2	MN	B	503	1/1	1.00	0.03	13,13,13,13	0
2	MN	B	504	1/1	1.00	0.03	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.