



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:55 PM UTC

PDB ID : 3ITY / pdb\_00003ity  
Title : Metal-free form of Pseudomonas stutzeri L-rhamnose isomerase  
Authors : Yoshida, H.; Yamaji, M.; Ishii, T.; Izumori, K.; Kamitori, S.  
Deposited on : 2009-08-28  
Resolution : 1.84 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

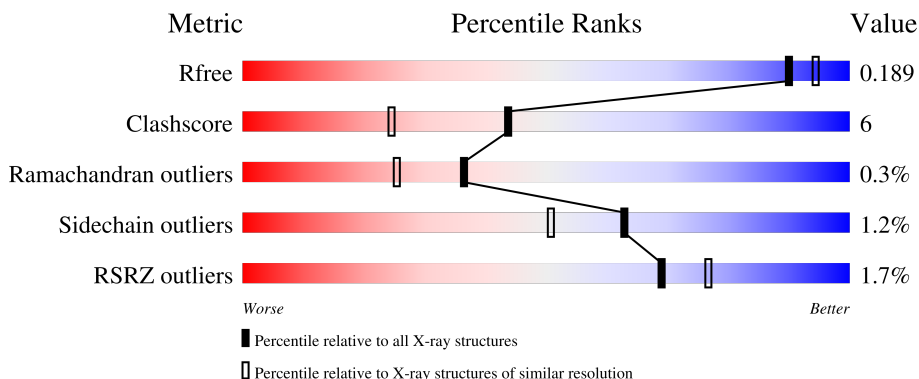
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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))
$R_{free}$	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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  $\geq 3$ , 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	438	 81% 14% .
1	B	438	 81% 15% .
1	C	438	 82% 15% .
1	D	438	 83% 12% .

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 15057 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
			Total	C	N	O	S			
1	A	421	Total 3260	C 2048	N 584	O 619	S 9	0	0	0
1	B	421	Total 3260	C 2048	N 584	O 619	S 9	0	0	0
1	C	428	Total 3301	C 2073	N 591	O 628	S 9	0	0	0
1	D	419	Total 3251	C 2042	N 582	O 618	S 9	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	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	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
C	431	GLY	-	expression tag	UNP Q75WH8
C	432	SER	-	expression tag	UNP Q75WH8

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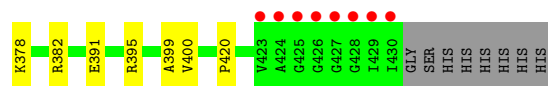
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Chain	Residue	Modelled	Actual	Comment	Reference
C	433	HIS	-	expression tag	UNP Q75WH8
C	434	HIS	-	expression tag	UNP Q75WH8
C	435	HIS	-	expression tag	UNP Q75WH8
C	436	HIS	-	expression tag	UNP Q75WH8
C	437	HIS	-	expression tag	UNP Q75WH8
C	438	HIS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

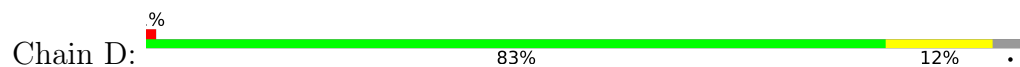
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	507	Total O 507 507	0	0
2	B	512	Total O 512 512	0	0
2	C	458	Total O 458 458	0	0
2	D	508	Total O 508 508	0	0





- Molecule 1: L-rhamnose isomerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.69Å 104.78Å 114.25Å 90.00° 107.98° 90.00°	Depositor
Resolution (Å)	46.94 – 1.84 46.94 – 1.84	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.94-1.84) 97.0 (46.94-1.84)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.77 (at 1.84Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.158 , 0.190 0.157 , 0.189	Depositor DCC
$R_{free}$ test set	14044 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.5	Xtrriage
Anisotropy	0.060	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15057	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.34	0/3332	0.82	7/4518 (0.2%)
1	B	0.33	0/3332	0.83	6/4518 (0.1%)
1	C	0.33	0/3373	0.80	5/4572 (0.1%)
1	D	0.34	0/3323	0.80	2/4505 (0.0%)
All	All	0.33	0/13360	0.81	20/18113 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	GLY	CA-C-N	6.72	126.98	119.32
1	B	246	GLY	C-N-CA	6.72	126.98	119.32
1	B	321	HIS	CA-C-N	6.69	126.73	119.90
1	B	321	HIS	C-N-CA	6.69	126.73	119.90
1	C	282	PHE	N-CA-C	6.03	119.72	110.20
1	C	191	ASN	N-CA-C	-5.70	99.23	108.41
1	C	246	GLY	CA-C-N	5.69	126.07	119.47
1	C	246	GLY	C-N-CA	5.69	126.07	119.47
1	A	401	ASP	CA-C-N	5.64	125.11	119.24
1	A	401	ASP	C-N-CA	5.64	125.11	119.24
1	A	246	GLY	CA-C-N	5.62	125.99	119.47
1	A	246	GLY	C-N-CA	5.62	125.99	119.47
1	B	282	PHE	N-CA-C	5.38	118.70	110.20
1	A	191	ASN	N-CA-C	-5.34	99.82	108.41
1	A	282	PHE	N-CA-C	5.33	118.91	109.96
1	C	227	PHE	N-CA-C	5.28	119.70	112.88
1	A	233	GLN	N-CA-C	5.25	118.84	112.23
1	D	282	PHE	N-CA-C	5.15	118.61	109.96
1	B	233	GLN	N-CA-C	5.13	118.70	112.23
1	D	233	GLN	N-CA-C	5.10	118.65	112.23

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	3260	0	3165	43	0
1	B	3260	0	3165	38	0
1	C	3301	0	3205	42	0
1	D	3251	0	3152	37	0
2	A	507	0	0	6	0
2	B	512	0	0	2	0
2	C	458	0	0	3	0
2	D	508	0	0	4	0
All	All	15057	0	12687	158	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 6.

All (158) 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:B:129:ASN:H	1:B:160:HIS:HE1	1.20	0.89
1:A:129:ASN:H	1:A:160:HIS:HE1	1.18	0.89
1:C:129:ASN:H	1:C:160:HIS:HE1	1.25	0.81
1:D:129:ASN:H	1:D:160:HIS:HE1	1.27	0.80
1:A:129:ASN:H	1:A:160:HIS:CE1	2.00	0.79
1:A:59:VAL:HG21	1:A:84:ASP:HB2	1.66	0.77
1:D:129:ASN:H	1:D:160:HIS:CE1	2.04	0.75
1:B:280:PHE:H	1:B:324:HIS:HD2	1.34	0.75
1:B:129:ASN:H	1:B:160:HIS:CE1	2.04	0.75
1:A:220:HIS:HE2	1:A:258:HIS:CE1	2.06	0.74
1:C:220:HIS:HE2	1:C:258:HIS:CE1	2.09	0.70
1:A:220:HIS:HE2	1:A:258:HIS:HE1	1.39	0.70
1:C:129:ASN:H	1:C:160:HIS:CE1	2.09	0.70
1:D:220:HIS:HE2	1:D:258:HIS:CE1	2.10	0.69
1:D:185:ASN:H	1:D:189:GLN:HE22	1.40	0.69
1:C:280:PHE:H	1:C:324:HIS:HD2	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:LYS:O	1:D:27:GLU:HG3	1.94	0.68
1:C:220:HIS:HE2	1:C:258:HIS:HE1	1.41	0.68
1:B:205:GLU:HA	1:B:208:LYS:HE2	1.76	0.68
1:B:185:ASN:H	1:B:189:GLN:HE22	1.42	0.67
1:C:210:LEU:HD11	1:C:216:LEU:HB2	1.76	0.67
1:A:59:VAL:HG21	1:A:84:ASP:CB	2.26	0.66
1:B:220:HIS:HE2	1:B:258:HIS:CE1	2.14	0.65
1:D:185:ASN:H	1:D:189:GLN:NE2	1.96	0.64
1:A:76:ARG:HD3	1:A:80:ASP:OD2	1.98	0.64
1:A:185:ASN:H	1:A:189:GLN:HE22	1.44	0.64
1:A:280:PHE:H	1:A:324:HIS:HD2	1.46	0.62
1:B:23:LYS:O	1:B:27:GLU:HG3	1.99	0.62
1:A:56:SER:O	1:A:59:VAL:HG12	2.00	0.62
1:A:217:PHE:HB3	1:A:252:LEU:HG	1.82	0.61
1:C:391:GLU:O	1:C:395:ARG:HG3	2.01	0.61
1:D:108:ASP:OD2	1:D:111:GLU:HG3	2.00	0.61
1:D:220:HIS:HE2	1:D:258:HIS:HE1	1.47	0.61
1:A:15:ASN:ND2	1:A:400:VAL:H	1.99	0.60
1:B:185:ASN:H	1:B:189:GLN:NE2	2.00	0.60
1:C:185:ASN:H	1:C:189:GLN:HE22	1.47	0.60
1:C:44:THR:O	1:C:48:GLU:HG3	2.01	0.60
1:D:15:ASN:ND2	1:D:400:VAL:H	2.01	0.59
1:A:5:ARG:HD2	1:A:83:ASP:O	2.03	0.59
1:B:220:HIS:HE2	1:B:258:HIS:HE1	1.48	0.59
1:A:185:ASN:H	1:A:189:GLN:NE2	2.00	0.59
1:A:23:LYS:O	1:A:27:GLU:HG3	2.03	0.59
1:B:54:VAL:HG23	1:B:95:THR:HB	1.83	0.59
1:D:217:PHE:HB3	1:D:252:LEU:HG	1.85	0.58
1:B:217:PHE:HB3	1:B:252:LEU:HG	1.86	0.58
1:C:48:GLU:CD	1:C:395:ARG:HH21	2.12	0.58
1:B:210:LEU:HD11	1:B:216:LEU:HB2	1.85	0.57
1:B:263:ASN:OD1	1:B:265:GLU:HG2	2.05	0.57
1:A:366:GLU:HG2	2:A:575:HOH:O	2.05	0.57
1:B:15:ASN:ND2	1:B:400:VAL:H	2.03	0.57
1:B:324:HIS:HE1	2:B:876:HOH:O	1.88	0.57
1:C:205:GLU:HA	1:C:208:LYS:HE2	1.86	0.57
1:A:210:LEU:HD11	1:A:216:LEU:HB2	1.88	0.56
1:B:315:ARG:HH11	1:B:315:ARG:HG3	1.71	0.56
1:C:217:PHE:HB3	1:C:252:LEU:HG	1.86	0.56
1:D:320:PHE:CE1	1:D:322:PRO:HG3	2.41	0.56
1:A:15:ASN:HD21	1:A:400:VAL:H	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ASN:H	1:C:189:GLN:NE2	2.04	0.56
1:B:414:ARG:O	1:B:418:GLU:HG3	2.06	0.55
1:D:193:THR:O	1:D:197:GLU:HG3	2.07	0.55
1:A:324:HIS:HE1	2:A:1576:HOH:O	1.90	0.55
1:C:361:LEU:O	1:C:365:GLN:HG3	2.07	0.55
1:A:193:THR:O	1:A:197:GLU:HG3	2.08	0.54
1:C:165:ILE:O	1:C:169:LYS:HG3	2.08	0.54
1:C:255:LEU:HD22	1:C:264:ILE:HD13	1.89	0.54
1:B:15:ASN:HD21	1:B:399:ALA:HA	1.73	0.54
1:B:311:ASP:OD1	1:B:315:ARG:NH1	2.41	0.54
1:C:7:ALA:HB1	1:C:9:ASP:OD1	2.08	0.53
1:C:15:ASN:HD21	1:C:399:ALA:HA	1.73	0.53
1:A:211:PRO:HD2	1:A:214:TRP:CG	2.44	0.53
1:A:263:ASN:OD1	1:A:265:GLU:HG2	2.09	0.53
1:D:59:VAL:HG12	1:D:75:PRO:HG3	1.91	0.53
1:D:361:LEU:O	1:D:365:GLN:HG3	2.09	0.53
1:C:23:LYS:O	1:C:27:GLU:HG3	2.08	0.52
1:B:211:PRO:HD2	1:B:214:TRP:CG	2.44	0.52
1:B:165:ILE:O	1:B:169:LYS:HG3	2.09	0.52
1:D:76:ARG:HD3	1:D:420:PRO:HD2	1.91	0.52
1:D:414:ARG:O	1:D:418:GLU:HG3	2.09	0.52
1:C:15:ASN:ND2	1:C:400:VAL:H	2.08	0.52
1:C:316:GLY:O	1:C:317:VAL:C	2.53	0.52
1:D:15:ASN:HD21	1:D:400:VAL:H	1.56	0.52
1:B:310:VAL:HG21	1:B:353:ALA:HB3	1.92	0.51
1:A:221:LYS:HA	1:A:257:HIS:HB3	1.92	0.51
1:D:66:PHE:O	1:D:67:ALA:HB2	2.10	0.51
1:D:15:ASN:HD21	1:D:399:ALA:HA	1.76	0.51
1:D:324:HIS:HE1	2:D:1594:HOH:O	1.93	0.51
1:A:414:ARG:O	1:A:418:GLU:HG3	2.12	0.50
1:D:280:PHE:H	1:D:324:HIS:HD2	1.59	0.50
1:A:165:ILE:O	1:A:169:LYS:HG3	2.12	0.50
1:B:321:HIS:N	1:B:322:PRO:HD3	2.26	0.49
1:A:59:VAL:HG22	1:A:59:VAL:O	2.13	0.49
1:B:361:LEU:O	1:B:365:GLN:HG3	2.12	0.48
1:C:324:HIS:HE1	2:C:1577:HOH:O	1.94	0.48
1:B:15:ASN:HD21	1:B:400:VAL:H	1.60	0.48
1:D:76:ARG:HD3	1:D:420:PRO:CD	2.43	0.48
1:D:221:LYS:HA	1:D:257:HIS:HB3	1.95	0.48
1:D:177:THR:HG23	1:D:252:LEU:HD12	1.97	0.47
1:A:166:GLU:HG2	2:A:1301:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:HE2	2:A:472:HOH:O	2.15	0.47
1:C:55:PRO:HD3	1:C:326:ILE:O	2.15	0.47
1:A:15:ASN:HD21	1:A:399:ALA:HA	1.80	0.47
1:B:193:THR:O	1:B:197:GLU:HG3	2.15	0.47
2:B:1551:HOH:O	1:C:301:ARG:HD3	2.14	0.47
1:C:108:ASP:OD2	1:C:110:LYS:HB2	2.14	0.47
1:C:193:THR:O	1:C:197:GLU:HG3	2.15	0.47
1:B:55:PRO:HD3	1:B:326:ILE:O	2.15	0.46
1:D:55:PRO:HD3	1:D:326:ILE:O	2.15	0.46
1:D:320:PHE:CZ	1:D:322:PRO:HG3	2.50	0.46
1:D:8:GLN:HG3	2:D:922:HOH:O	2.14	0.46
1:D:108:ASP:OD2	1:D:110:LYS:HB2	2.16	0.46
2:A:779:HOH:O	1:D:382:ARG:HD3	2.16	0.46
1:A:191:ASN:ND2	1:C:315:ARG:NH1	2.64	0.46
1:C:211:PRO:HD2	1:C:214:TRP:CG	2.50	0.46
1:B:255:LEU:C	1:B:255:LEU:HD13	2.41	0.46
1:C:68:ARG:HH12	1:C:70:PRO:HB3	1.81	0.46
1:A:301:ARG:HD3	2:D:1626:HOH:O	2.15	0.45
1:D:13:ARG:HH21	1:D:13:ARG:HG3	1.81	0.45
1:B:68:ARG:HH12	1:B:70:PRO:HB3	1.82	0.45
1:D:263:ASN:OD1	1:D:265:GLU:HG2	2.16	0.45
1:D:255:LEU:C	1:D:255:LEU:HD23	2.42	0.45
1:D:129:ASN:N	1:D:160:HIS:HE1	2.06	0.44
1:A:191:ASN:ND2	1:C:315:ARG:HH12	2.14	0.44
1:B:7:ALA:HB1	1:B:9:ASP:OD1	2.17	0.44
1:C:76:ARG:HD3	1:C:420:PRO:HD2	1.99	0.44
1:B:340:ILE:HG21	1:B:402:PRO:HB2	2.00	0.44
1:B:221:LYS:HA	1:B:257:HIS:HB3	1.98	0.44
1:B:382:ARG:HD3	2:C:627:HOH:O	2.17	0.43
1:A:255:LEU:C	1:A:255:LEU:HD23	2.43	0.43
1:A:137:GLN:HG2	1:A:156:GLN:HE22	1.83	0.43
1:C:221:LYS:HA	1:C:257:HIS:HB3	1.99	0.43
1:C:263:ASN:OD1	1:C:265:GLU:HG2	2.18	0.43
1:C:66:PHE:O	1:C:67:ALA:HB2	2.18	0.43
1:C:68:ARG:NH1	1:C:70:PRO:HB3	2.33	0.43
1:C:255:LEU:C	1:C:255:LEU:HD13	2.43	0.43
1:A:55:PRO:HD3	1:A:326:ILE:O	2.19	0.43
1:A:201:SER:HB3	2:A:1330:HOH:O	2.18	0.42
1:C:115:ARG:HA	1:C:115:ARG:HD2	1.84	0.42
1:C:289:ASP:HB3	2:C:1642:HOH:O	2.19	0.42
1:A:76:ARG:HH11	1:A:419:ARG:HG2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:LYS:O	1:C:382:ARG:HG3	2.19	0.42
1:B:255:LEU:O	1:B:258:HIS:HD2	2.03	0.42
1:A:318:LYS:N	1:A:318:LYS:HD2	2.35	0.42
1:D:68:ARG:HH22	1:D:70:PRO:HB3	1.85	0.42
1:A:137:GLN:HG2	1:A:156:GLN:NE2	2.35	0.42
1:C:221:LYS:HE2	1:C:223:TYR:O	2.20	0.41
1:D:54:VAL:HG13	1:D:95:THR:HB	2.01	0.41
1:A:54:VAL:HG23	1:A:95:THR:HB	2.02	0.41
1:A:66:PHE:O	1:A:67:ALA:HB2	2.19	0.41
1:C:15:ASN:HD21	1:C:400:VAL:H	1.66	0.41
1:A:129:ASN:N	1:A:160:HIS:HE1	2.01	0.41
1:B:129:ASN:N	1:B:160:HIS:HE1	2.02	0.41
1:B:180:ILE:HD12	1:B:182:ASP:CG	2.46	0.41
1:B:386:GLU:N	1:B:387:PRO:CD	2.84	0.41
1:A:361:LEU:O	1:A:365:GLN:HG3	2.21	0.41
1:D:340:ILE:HG21	1:D:402:PRO:HB2	2.02	0.41
1:C:180:ILE:HD12	1:C:182:ASP:CG	2.46	0.40
1:B:66:PHE:O	1:B:67:ALA:HB2	2.21	0.40
1:D:160:HIS:HD2	2:D:1584:HOH:O	2.03	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	419/438 (96%)	410 (98%)	8 (2%)	1 (0%)	43 34
1	B	419/438 (96%)	408 (97%)	10 (2%)	1 (0%)	43 34
1	C	426/438 (97%)	414 (97%)	10 (2%)	2 (0%)	24 12
1	D	417/438 (95%)	405 (97%)	11 (3%)	1 (0%)	43 34
All	All	1681/1752 (96%)	1637 (97%)	39 (2%)	5 (0%)	36 25

All (5) Ramachandran outliers are listed below:

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

### 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	330/341 (97%)	324 (98%)	6 (2%)	51 35
1	B	330/341 (97%)	326 (99%)	4 (1%)	63 51
1	C	333/341 (98%)	331 (99%)	2 (1%)	78 72
1	D	329/341 (96%)	325 (99%)	4 (1%)	63 51
All	All	1322/1364 (97%)	1306 (99%)	16 (1%)	63 51

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	SER
1	A	124	ASP
1	A	318	LYS
1	A	374	THR
1	A	377	LEU
1	A	422	SER
1	B	99	SER
1	B	110	LYS
1	B	354	LEU
1	B	374	THR
1	C	99	SER
1	C	374	THR
1	D	59	VAL
1	D	99	SER
1	D	124	ASP

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Mol	Chain	Res	Type
1	D	374	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	160	HIS
1	A	189	GLN
1	A	191	ASN
1	A	243	GLN
1	A	258	HIS
1	A	324	HIS
1	A	344	ASN
1	A	365	GLN
1	B	8	GLN
1	B	15	ASN
1	B	160	HIS
1	B	189	GLN
1	B	258	HIS
1	B	321	HIS
1	B	324	HIS
1	B	344	ASN
1	C	8	GLN
1	C	15	ASN
1	C	150	ASN
1	C	160	HIS
1	C	189	GLN
1	C	258	HIS
1	C	324	HIS
1	C	344	ASN
1	C	352	GLN
1	C	365	GLN
1	D	15	ASN
1	D	139	HIS
1	D	160	HIS
1	D	189	GLN
1	D	258	HIS
1	D	324	HIS
1	D	344	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	421/438 (96%)	-0.45	2 (0%) 87 92	7, 11, 23, 35	0
1	B	421/438 (96%)	-0.31	5 (1%) 76 82	7, 12, 25, 43	0
1	C	428/438 (97%)	-0.03	18 (4%) 40 43	8, 15, 33, 55	0
1	D	419/438 (95%)	-0.35	4 (0%) 79 86	7, 12, 26, 43	0
All	All	1689/1752 (96%)	-0.28	29 (1%) 69 77	7, 13, 27, 55	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	430	ILE	8.4
1	C	427	GLY	7.3
1	B	424	ALA	7.1
1	D	421	ALA	6.4
1	C	429	ILE	5.7
1	C	428	GLY	5.5
1	C	319	GLY	4.4
1	A	424	ALA	3.8
1	D	420	PRO	3.7
1	C	424	ALA	3.7
1	C	317	VAL	3.7
1	C	316	GLY	3.5
1	B	316	GLY	3.4
1	C	425	GLY	3.3
1	C	426	GLY	3.3
1	C	314	ALA	3.3
1	A	423	VAL	2.9
1	C	318	LYS	2.7
1	B	423	VAL	2.7
1	B	315	ARG	2.7
1	C	315	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	321	HIS	2.4
1	C	320	PHE	2.3
1	C	423	VAL	2.3
1	D	110	LYS	2.2
1	D	3	GLU	2.2
1	C	110	LYS	2.1
1	B	8	GLN	2.0
1	C	367	ASP	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.