



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:04 PM UTC

PDB ID : 3IUI / pdb_00003iui
Title : Zn²⁺-bound form of Pseudomonas stutzeri L-rhamnose isomerase
Authors : Yoshida, H.; Yamaji, M.; Ishii, T.; Izumori, K.; Kamitori, S.
Deposited on : 2009-08-31
Resolution : 2.30 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

<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	:	4-5-2 with Phenix2.0
Xtriage (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

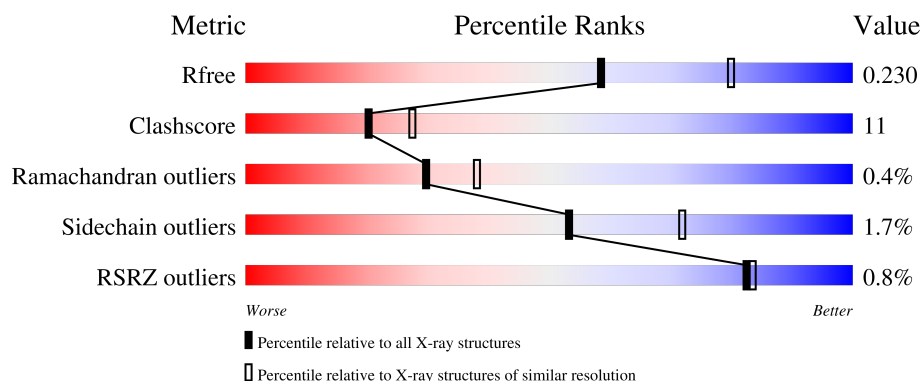
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	438	% 74% 21% • 5%
1	B	438	75% 20% 5%
1	C	438	78% 16% • •
1	D	438	% 76% 19% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13712 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	418	Total	C	N	O	S	0	0	0
			3242	2037	581	615	9			
1	B	418	Total	C	N	O	S	0	0	0
			3242	2037	581	615	9			
1	C	420	Total	C	N	O	S	0	0	0
			3255	2045	583	618	9			
1	D	420	Total	C	N	O	S	0	0	0
			3255	2045	583	618	9			

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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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 ZINC ION (CCD ID: ZN) (formula: Zn).

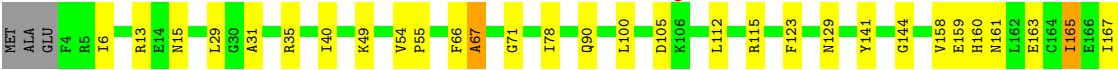
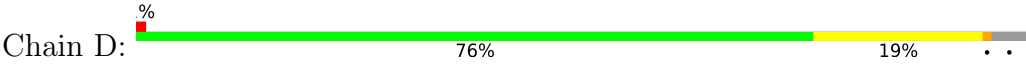
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	151	Total O 151 151	0	0
3	B	168	Total O 168 168	0	0
3	C	198	Total O 198 198	0	0
3	D	193	Total O 193 193	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, α , β , γ	78.69Å 104.83Å 101.77Å 90.00° 102.98° 90.00°	Depositor
Resolution (Å)	38.81 – 2.30 38.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.0 (38.81-2.30) 94.0 (38.81-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.71 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.182 , 0.230 0.182 , 0.230	Depositor DCC
R_{free} test set	6816 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	24.3	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13712	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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

5.1 Standard geometry

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

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	0.38	0/3314	0.85	5/4493 (0.1%)
1	B	0.38	0/3314	0.88	5/4493 (0.1%)
1	C	0.40	0/3327	0.88	4/4511 (0.1%)
1	D	0.42	0/3327	0.89	6/4511 (0.1%)
All	All	0.40	0/13282	0.87	20/18008 (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	D	246	GLY	CA-C-N	7.04	127.35	119.32
1	D	246	GLY	C-N-CA	7.04	127.35	119.32
1	C	191	ASN	N-CA-C	-6.57	97.84	108.41
1	C	246	GLY	CA-C-N	6.36	126.27	119.28
1	C	246	GLY	C-N-CA	6.36	126.27	119.28
1	B	246	GLY	CA-C-N	6.34	127.76	119.84
1	B	246	GLY	C-N-CA	6.34	127.76	119.84
1	D	71	GLY	N-CA-C	-6.19	104.09	112.57
1	A	401	ASP	CA-C-N	6.05	125.53	119.24
1	A	401	ASP	C-N-CA	6.05	125.53	119.24
1	A	233	GLN	N-CA-C	5.89	118.94	111.69
1	C	334	ASP	N-CA-C	-5.88	100.72	109.42
1	B	245	LEU	N-CA-C	5.81	117.61	111.28
1	B	227	PHE	N-CA-C	5.47	120.07	113.17
1	D	334	ASP	N-CA-C	-5.44	101.37	109.42
1	B	191	ASN	N-CA-C	-5.36	99.03	108.20
1	A	246	GLY	CA-C-N	5.33	125.65	119.47
1	A	246	GLY	C-N-CA	5.33	125.65	119.47
1	D	227	PHE	N-CA-C	5.26	119.67	112.88
1	D	67	ALA	N-CA-C	5.15	116.26	108.07

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	3242	0	3146	80	0
1	B	3242	0	3146	65	0
1	C	3255	0	3160	68	0
1	D	3255	0	3160	78	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	151	0	0	2	0
3	B	168	0	0	3	0
3	C	198	0	0	3	0
3	D	193	0	0	4	0
All	All	13712	0	12612	290	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 (290) 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:C:78:ILE:HD12	1:C:105:ASP:HB3	1.31	1.12
1:B:102:ILE:HD11	1:B:126:MET:HE3	1.37	1.06
1:A:78:ILE:HD12	1:A:105:ASP:HB3	1.39	1.02
1:B:78:ILE:HD12	1:B:105:ASP:HB3	1.42	1.00
1:D:78:ILE:HD12	1:D:105:ASP:HB3	1.46	0.98
1:A:29:LEU:HD23	1:A:388:ILE:HD13	1.50	0.94
1:A:6:ILE:HD11	1:A:87:VAL:HG13	1.49	0.93
1:C:129:ASN:H	1:C:160:HIS:HE1	1.16	0.89
1:A:29:LEU:HD23	1:A:388:ILE:CD1	2.04	0.87
1:A:40:ILE:HD11	1:A:388:ILE:HD11	1.57	0.86
1:D:196:PHE:CE1	1:D:241:ILE:HD11	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:336:ILE:HD13	1:D:412:ARG:NH2	1.94	0.83
1:A:336:ILE:HD13	1:A:412:ARG:NH2	1.93	0.81
1:C:158:VAL:HA	1:C:206:ILE:HD11	1.60	0.81
1:D:196:PHE:HE1	1:D:241:ILE:HD11	1.43	0.81
1:C:129:ASN:H	1:C:160:HIS:CE1	1.98	0.80
1:B:336:ILE:HD13	1:B:412:ARG:NH2	1.96	0.79
1:A:210:LEU:HD11	1:A:216:LEU:HB2	1.63	0.78
1:C:255:LEU:HG	1:C:280:PHE:CE1	2.19	0.78
1:B:280:PHE:CE2	1:B:309:LEU:HD21	2.19	0.77
1:D:40:ILE:HD11	1:D:388:ILE:HD11	1.66	0.76
1:B:220:HIS:HE2	1:B:258:HIS:HE1	1.30	0.76
1:B:280:PHE:HE2	1:B:309:LEU:HD21	1.51	0.74
1:B:220:HIS:HE2	1:B:258:HIS:CE1	2.05	0.74
1:D:165:ILE:HD13	1:D:214:TRP:CZ3	2.23	0.74
1:C:40:ILE:HD11	1:C:388:ILE:CD1	2.18	0.74
1:A:129:ASN:H	1:A:160:HIS:HE1	1.36	0.73
1:B:180:ILE:HD12	1:B:182:ASP:CG	2.13	0.72
1:C:210:LEU:HD11	1:C:216:LEU:HB2	1.72	0.72
1:C:99:SER:OG	1:C:325:MET:HE2	1.89	0.72
1:C:180:ILE:HD13	1:C:180:ILE:H	1.55	0.72
1:D:40:ILE:HD11	1:D:388:ILE:CD1	2.20	0.71
1:B:59:VAL:HG21	1:B:84:ASP:HB2	1.71	0.71
1:B:252:LEU:HD21	1:B:281:HIS:CD2	2.27	0.70
1:D:180:ILE:HD12	1:D:182:ASP:CG	2.17	0.69
1:C:6:ILE:H	1:C:90:GLN:HE22	1.39	0.69
1:C:318:LYS:HE3	1:C:318:LYS:HA	1.74	0.69
1:A:336:ILE:HD13	1:A:412:ARG:HH22	1.55	0.69
1:D:272:ILE:HD11	1:D:277:LEU:CD2	2.21	0.69
1:D:78:ILE:HD13	1:D:112:LEU:HD21	1.75	0.68
1:A:235:TRP:NE1	1:A:267:ILE:HD12	2.08	0.68
1:A:40:ILE:HD11	1:A:388:ILE:CD1	2.23	0.68
1:D:158:VAL:HA	1:D:206:ILE:HD11	1.76	0.68
1:C:40:ILE:HD11	1:C:388:ILE:HG13	1.76	0.67
1:D:272:ILE:HD11	1:D:277:LEU:HD23	1.76	0.67
1:A:255:LEU:HD12	1:A:264:ILE:HD13	1.75	0.67
1:B:235:TRP:CD1	1:B:267:ILE:HD12	2.30	0.66
1:D:217:PHE:HB3	1:D:252:LEU:HG	1.78	0.66
1:D:336:ILE:HD13	1:D:412:ARG:HH22	1.60	0.66
1:A:40:ILE:CD1	1:A:388:ILE:HD11	2.27	0.66
1:A:129:ASN:H	1:A:160:HIS:CE1	2.15	0.65
1:A:180:ILE:HD13	1:A:180:ILE:H	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ILE:HD13	3:A:515:HOH:O	1.96	0.65
1:B:252:LEU:HD21	1:B:281:HIS:CG	2.32	0.64
1:C:414:ARG:O	1:C:418:GLU:HG3	1.98	0.64
1:D:284:ASP:HB3	1:D:297:ILE:HD13	1.79	0.64
1:D:199:TYR:HE1	1:D:241:ILE:HD12	1.63	0.64
1:B:76:ARG:NH2	1:B:420:PRO:HG2	2.14	0.63
1:B:108:ASP:OD2	1:B:110:LYS:HG3	1.98	0.63
1:B:282:PHE:HB2	1:B:326:ILE:HD13	1.81	0.63
1:C:180:ILE:HD13	3:C:519:HOH:O	2.00	0.62
1:D:200:LEU:HD21	1:D:241:ILE:HD13	1.82	0.62
1:D:29:LEU:HD23	1:D:388:ILE:CD1	2.30	0.62
1:A:382:ARG:HD3	3:A:439:HOH:O	2.00	0.61
1:A:220:HIS:HE2	1:A:258:HIS:CE1	2.18	0.61
1:D:165:ILE:HD13	1:D:214:TRP:CE3	2.35	0.61
1:D:361:LEU:O	1:D:365:GLN:HG3	2.01	0.61
1:B:129:ASN:H	1:B:160:HIS:CE1	2.18	0.61
1:A:29:LEU:CD2	1:A:388:ILE:HD13	2.29	0.61
1:C:255:LEU:HG	1:C:280:PHE:CZ	2.36	0.61
1:D:158:VAL:HG13	1:D:206:ILE:HD13	1.82	0.61
1:B:252:LEU:HD11	1:B:281:HIS:NE2	2.16	0.61
1:D:272:ILE:HD12	1:D:320:PHE:CD1	2.35	0.60
1:A:23:LYS:O	1:A:27:GLU:HG3	2.02	0.60
1:A:240:LEU:HD13	1:C:274:PHE:CE2	2.36	0.60
1:D:159:GLU:O	1:D:163:GLU:HG3	2.03	0.59
1:B:129:ASN:H	1:B:160:HIS:HE1	1.50	0.59
1:C:29:LEU:HD23	1:C:388:ILE:HD11	1.85	0.59
1:B:263:ASN:OD1	1:B:265:GLU:HG2	2.02	0.59
1:D:272:ILE:HG22	1:D:317:VAL:HG11	1.84	0.58
1:C:161:ASN:HB2	1:C:206:ILE:HD12	1.86	0.58
1:C:33:LEU:CD1	1:C:40:ILE:HD13	2.32	0.58
1:C:255:LEU:HG	1:C:280:PHE:HE1	1.65	0.58
1:D:268:VAL:O	1:D:272:ILE:HG12	2.04	0.58
1:A:44:THR:O	1:A:48:GLU:HG3	2.03	0.58
1:B:59:VAL:HG13	1:B:75:PRO:HG3	1.85	0.58
1:A:221:LYS:HA	1:A:257:HIS:HB3	1.86	0.57
1:B:154:ARG:O	1:B:158:VAL:HG23	2.04	0.57
1:C:40:ILE:HD11	1:C:388:ILE:CG1	2.34	0.57
1:C:33:LEU:HD12	1:C:40:ILE:HD13	1.86	0.57
1:A:255:LEU:CD1	1:A:264:ILE:HD13	2.35	0.57
1:D:129:ASN:H	1:D:160:HIS:HE1	1.51	0.57
1:A:102:ILE:HG23	1:A:103:PRO:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:LEU:O	1:A:365:GLN:HG3	2.05	0.56
1:C:108:ASP:OD2	1:C:110:LYS:HB2	2.04	0.56
1:D:185:ASN:H	1:D:189:GLN:HE22	1.53	0.56
1:D:29:LEU:HD23	1:D:388:ILE:HD13	1.86	0.56
1:B:102:ILE:HD11	1:B:126:MET:CE	2.24	0.56
1:D:207:TYR:O	1:D:210:LEU:HB2	2.05	0.56
1:D:272:ILE:HD13	1:D:277:LEU:HB3	1.86	0.56
1:D:199:TYR:CE1	1:D:241:ILE:HD12	2.40	0.56
1:B:102:ILE:N	1:B:102:ILE:HD12	2.21	0.56
1:A:185:ASN:H	1:A:189:GLN:HE22	1.53	0.56
1:C:263:ASN:OD1	1:C:265:GLU:HG2	2.06	0.56
1:A:375:GLU:O	1:A:379:ARG:HG3	2.06	0.55
1:D:378:LYS:O	1:D:382:ARG:HG3	2.06	0.55
1:A:6:ILE:HD11	1:A:87:VAL:CG1	2.32	0.55
1:A:202:ALA:O	1:A:206:ILE:HD12	2.05	0.55
1:D:163:GLU:O	1:D:167:ILE:HG12	2.07	0.55
1:A:29:LEU:HD23	1:A:388:ILE:HD11	1.87	0.55
1:D:123:PHE:CG	1:D:171:ILE:HD12	2.41	0.55
1:B:336:ILE:HD13	1:B:412:ARG:HH21	1.72	0.55
1:C:78:ILE:HD13	1:C:112:LEU:HD21	1.88	0.55
1:A:55:PRO:HD3	1:A:326:ILE:O	2.07	0.54
1:A:78:ILE:HD13	1:A:112:LEU:HD22	1.89	0.54
1:B:185:ASN:H	1:B:189:GLN:HE22	1.55	0.54
1:B:6:ILE:HB	1:B:90:GLN:NE2	2.22	0.54
1:B:235:TRP:NE1	1:B:267:ILE:HD12	2.24	0.53
1:D:297:ILE:N	1:D:297:ILE:HD12	2.24	0.53
1:D:193:THR:O	1:D:197:GLU:HG3	2.09	0.53
1:B:55:PRO:HD3	1:B:326:ILE:O	2.08	0.52
1:C:325:MET:HE1	3:C:455:HOH:O	2.08	0.52
1:D:185:ASN:H	1:D:189:GLN:NE2	2.07	0.52
1:D:221:LYS:HA	1:D:257:HIS:HB3	1.90	0.52
1:A:220:HIS:HE2	1:A:258:HIS:HE1	1.58	0.52
1:C:76:ARG:HD3	1:C:420:PRO:HD2	1.92	0.52
1:D:272:ILE:HD11	1:D:277:LEU:HD22	1.92	0.52
1:A:325:MET:HG2	1:A:326:ILE:N	2.25	0.52
1:D:336:ILE:HD11	3:D:519:HOH:O	2.09	0.52
1:B:49:LYS:HE2	3:B:547:HOH:O	2.09	0.51
1:B:205:GLU:HA	1:B:208:LYS:HE2	1.93	0.51
1:D:6:ILE:H	1:D:90:GLN:HE22	1.59	0.51
1:D:31:ALA:O	1:D:35:ARG:HG3	2.10	0.51
1:A:414:ARG:O	1:A:418:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ILE:HD12	1:B:336:ILE:N	2.25	0.51
1:C:158:VAL:CA	1:C:206:ILE:HD11	2.38	0.51
1:C:311:ASP:O	1:C:315:ARG:HG3	2.10	0.51
1:A:235:TRP:CD1	1:A:267:ILE:HD12	2.45	0.51
1:A:78:ILE:HD13	1:A:112:LEU:CD2	2.41	0.51
1:A:6:ILE:N	1:A:6:ILE:HD12	2.26	0.51
1:A:264:ILE:HD12	1:A:301:ARG:HD2	1.93	0.51
1:B:185:ASN:H	1:B:189:GLN:NE2	2.08	0.50
1:C:129:ASN:N	1:C:160:HIS:HE1	1.95	0.50
1:B:7:ALA:HB3	1:B:10:VAL:HG23	1.91	0.50
1:D:158:VAL:HG13	1:D:206:ILE:CD1	2.40	0.50
1:A:158:VAL:HG22	1:A:206:ILE:HD11	1.94	0.50
1:B:361:LEU:O	1:B:365:GLN:HG3	2.12	0.50
1:C:388:ILE:HD13	1:C:388:ILE:N	2.27	0.50
1:C:99:SER:CB	1:C:325:MET:HE2	2.41	0.50
1:D:221:LYS:HE2	1:D:223:TYR:O	2.12	0.50
1:A:185:ASN:H	1:A:189:GLN:NE2	2.09	0.49
1:B:336:ILE:HD13	1:B:412:ARG:HH22	1.75	0.49
1:C:123:PHE:CG	1:C:171:ILE:HD12	2.46	0.49
1:D:129:ASN:H	1:D:160:HIS:CE1	2.29	0.49
1:B:336:ILE:HD11	3:B:494:HOH:O	2.12	0.49
1:A:57:TRP:CE3	1:A:101:HIS:HB2	2.48	0.49
1:A:180:ILE:HD13	1:A:180:ILE:N	2.28	0.49
1:A:411:TYR:O	1:A:415:VAL:HG22	2.12	0.49
1:D:78:ILE:HD13	1:D:112:LEU:CD2	2.40	0.49
1:B:23:LYS:O	1:B:27:GLU:HG3	2.12	0.49
1:C:55:PRO:HD3	1:C:326:ILE:O	2.13	0.49
1:B:7:ALA:HB1	1:B:9:ASP:OD1	2.13	0.49
1:A:222:MET:CE	1:A:259:ALA:HB2	2.44	0.48
1:B:108:ASP:OD2	1:B:110:LYS:HE2	2.12	0.48
1:B:342:SER:O	1:B:346:ILE:HG12	2.14	0.48
1:D:13:ARG:HG3	1:D:13:ARG:HH11	1.77	0.48
1:A:17:ARG:HG3	1:A:17:ARG:HH11	1.79	0.48
1:A:223:TYR:O	1:A:224:GLU:HB3	2.14	0.48
1:C:65:ARG:HG2	3:D:558:HOH:O	2.13	0.48
1:A:72:THR:O	1:A:412:ARG:HD2	2.13	0.48
1:B:221:LYS:O	1:B:233:GLN:HA	2.14	0.48
1:C:325:MET:CE	3:C:455:HOH:O	2.62	0.48
1:A:165:ILE:HD13	1:A:176:LEU:HB2	1.95	0.48
1:A:255:LEU:HD23	1:A:283:ASN:O	2.14	0.48
1:A:255:LEU:HD13	1:A:280:PHE:HZ	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ILE:HD13	1:C:112:LEU:CD2	2.43	0.47
1:C:419:ARG:HA	1:C:420:PRO:HD3	1.80	0.47
1:A:371:LEU:O	1:A:374:THR:HG22	2.14	0.47
1:C:330:HIS:CD2	1:C:338:SER:HB3	2.50	0.47
1:C:334:ASP:HB3	1:C:337:GLU:HG3	1.97	0.47
1:A:7:ALA:HB1	1:A:9:ASP:OD1	2.14	0.47
1:A:386:GLU:HB3	1:A:387:PRO:HD3	1.96	0.47
1:C:185:ASN:H	1:C:189:GLN:HE22	1.61	0.47
1:A:106:LYS:NZ	1:A:163:GLU:OE2	2.44	0.47
1:C:78:ILE:CD1	1:C:105:ASP:HB3	2.23	0.47
1:D:237:THR:O	1:D:241:ILE:HG12	2.14	0.47
1:A:336:ILE:N	1:A:336:ILE:HD12	2.30	0.47
1:A:336:ILE:CD1	1:A:412:ARG:HH22	2.25	0.47
1:D:336:ILE:HD12	1:D:336:ILE:N	2.30	0.46
1:A:78:ILE:HG23	1:A:79:PHE:N	2.30	0.46
1:B:108:ASP:CG	1:B:110:LYS:HG3	2.40	0.46
1:C:78:ILE:HD12	1:C:105:ASP:CB	2.23	0.46
1:D:256:GLY:H	1:D:283:ASN:HD21	1.63	0.46
1:D:281:HIS:HA	1:D:325:MET:O	2.15	0.46
1:A:165:ILE:HD11	1:A:176:LEU:HD22	1.98	0.46
1:A:92:THR:CG2	1:A:340:ILE:HG23	2.46	0.46
1:C:158:VAL:HG13	1:C:206:ILE:HD13	1.97	0.46
1:A:6:ILE:HB	1:A:90:GLN:NE2	2.31	0.45
1:C:78:ILE:HD11	1:C:100:LEU:HD22	1.97	0.45
1:A:165:ILE:HD11	1:A:176:LEU:CD2	2.47	0.45
1:B:6:ILE:HB	1:B:90:GLN:HE22	1.81	0.45
1:C:211:PRO:HD2	1:C:214:TRP:CG	2.51	0.45
1:B:315:ARG:HB3	1:B:315:ARG:HH11	1.81	0.45
1:D:49:LYS:HE2	3:D:510:HOH:O	2.17	0.45
1:C:29:LEU:HD23	1:C:388:ILE:CD1	2.45	0.45
1:A:194:ARG:O	1:A:198:ARG:HG3	2.17	0.45
1:B:43:VAL:O	1:B:47:VAL:HG23	2.17	0.45
1:D:66:PHE:O	1:D:67:ALA:HB2	2.17	0.45
1:D:158:VAL:CA	1:D:206:ILE:HD11	2.46	0.45
1:D:382:ARG:HD3	3:D:568:HOH:O	2.15	0.45
1:D:388:ILE:HD13	1:D:388:ILE:N	2.32	0.44
1:A:235:TRP:CE2	1:A:267:ILE:HD12	2.51	0.44
1:D:200:LEU:CD2	1:D:241:ILE:HD13	2.47	0.44
1:B:15:ASN:HD21	1:B:399:ALA:HA	1.82	0.44
1:C:386:GLU:HB3	1:C:387:PRO:HD3	1.99	0.44
1:B:129:ASN:C	1:B:129:ASN:OD1	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:LYS:HE3	1:C:110:LYS:HB3	1.89	0.44
1:B:131:PHE:HA	3:B:582:HOH:O	2.18	0.44
1:B:411:TYR:O	1:B:415:VAL:HG22	2.18	0.44
1:C:76:ARG:NH1	1:C:419:ARG:HG2	2.33	0.44
1:C:187:PRO:HG3	1:C:228:TYR:CE1	2.53	0.44
1:B:391:GLU:OE2	1:B:395:ARG:NE	2.49	0.44
1:C:147:SER:HB3	1:C:199:TYR:HB2	1.98	0.44
1:D:40:ILE:HD11	1:D:388:ILE:HD12	1.99	0.44
1:C:54:VAL:HG13	1:C:95:THR:HB	2.00	0.43
1:C:217:PHE:HB3	1:C:252:LEU:HD22	2.00	0.43
1:C:9:ASP:OD2	1:C:10:VAL:N	2.51	0.43
1:D:180:ILE:HD12	1:D:182:ASP:CB	2.49	0.43
1:A:282:PHE:CD1	1:A:346:ILE:HD12	2.54	0.43
1:C:161:ASN:CB	1:C:206:ILE:HD12	2.49	0.43
1:A:263:ASN:OD1	1:A:265:GLU:HG2	2.18	0.43
1:B:134:ALA:O	1:B:137:GLN:HB2	2.17	0.43
1:B:378:LYS:O	1:B:382:ARG:HG3	2.19	0.43
1:C:80:ASP:O	1:C:83:ASP:HB2	2.19	0.43
1:C:340:ILE:HG21	1:C:402:PRO:HB2	2.00	0.43
1:D:180:ILE:HD12	1:D:182:ASP:HB2	2.00	0.43
1:D:263:ASN:OD1	1:D:265:GLU:HG2	2.18	0.43
1:D:29:LEU:HD23	1:D:388:ILE:HD11	1.98	0.43
1:D:55:PRO:HD3	1:D:326:ILE:O	2.18	0.43
1:D:165:ILE:HD12	1:D:210:LEU:HD12	2.00	0.43
1:C:194:ARG:O	1:C:198:ARG:HG3	2.19	0.43
1:C:221:LYS:HA	1:C:257:HIS:HB3	2.00	0.43
1:D:283:ASN:C	1:D:283:ASN:HD22	2.26	0.43
1:C:76:ARG:HD3	1:C:420:PRO:CD	2.49	0.42
1:C:180:ILE:HD13	1:C:180:ILE:N	2.28	0.42
1:D:115:ARG:HD2	1:D:115:ARG:HA	1.70	0.42
1:D:272:ILE:HD12	1:D:320:PHE:CE1	2.55	0.42
1:A:5:ARG:HB2	1:A:6:ILE:HD12	2.02	0.42
1:A:255:LEU:O	1:A:258:HIS:HD2	2.03	0.42
1:D:165:ILE:O	1:D:169:LYS:HG3	2.19	0.42
1:A:193:THR:O	1:A:197:GLU:HG3	2.19	0.42
1:B:193:THR:O	1:B:197:GLU:HG3	2.20	0.42
1:D:161:ASN:HB2	1:D:206:ILE:HD12	2.02	0.42
1:A:202:ALA:O	1:A:206:ILE:CD1	2.68	0.41
1:A:336:ILE:N	1:A:336:ILE:CD1	2.83	0.41
1:B:221:LYS:HA	1:B:257:HIS:HB3	2.01	0.41
1:C:102:ILE:HG23	1:C:103:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ILE:CD1	1:D:388:ILE:HD11	2.41	0.41
1:A:100:LEU:HD13	1:A:123:PHE:HD2	1.85	0.41
1:D:310:VAL:HG21	1:D:353:ALA:CB	2.50	0.41
1:B:78:ILE:O	1:B:82:LEU:HG	2.20	0.41
1:A:92:THR:HG22	1:A:340:ILE:HG23	2.01	0.41
1:B:326:ILE:HD11	1:B:346:ILE:HG13	2.03	0.41
1:D:221:LYS:O	1:D:233:GLN:HA	2.20	0.41
1:A:342:SER:O	1:A:346:ILE:HG12	2.20	0.41
1:C:40:ILE:HD11	1:C:388:ILE:HD11	1.98	0.41
1:C:185:ASN:H	1:C:189:GLN:NE2	2.18	0.41
1:A:181:GLY:O	1:A:182:ASP:C	2.64	0.41
1:A:242:ALA:HB1	1:A:276:LYS:HD2	2.01	0.41
1:B:281:HIS:HA	1:B:325:MET:O	2.21	0.41
1:B:174:LYS:O	1:B:214:TRP:HA	2.21	0.41
1:D:311:ASP:OD2	1:D:315:ARG:HD3	2.21	0.41
1:A:73:GLY:CA	1:A:416:ALA:HA	2.51	0.40
1:B:199:TYR:CE1	1:B:203:MET:HG3	2.56	0.40
1:B:386:GLU:N	1:B:387:PRO:CD	2.84	0.40
1:B:59:VAL:HG11	1:B:81:LYS:HA	2.04	0.40
1:B:150:ASN:HD21	1:B:152:ALA:HB3	1.85	0.40
1:B:386:GLU:HB3	1:B:387:PRO:HD3	2.04	0.40
1:C:102:ILE:CG2	1:C:103:PRO:HA	2.51	0.40
1:A:158:VAL:HG22	1:A:206:ILE:CD1	2.51	0.40
1:D:322:PRO:HB2	1:D:324:HIS:CE1	2.56	0.40
1:B:102:ILE:CG2	1:B:103:PRO:HA	2.51	0.40
1:B:334:ASP:HB3	1:B:337:GLU:HG3	2.02	0.40
1:D:15:ASN:CG	1:D:400:VAL:HG23	2.47	0.40
1:D:78:ILE:CD1	1:D:100:LEU:HD22	2.52	0.40
1:D:141:TYR:HA	1:D:144:GLY:O	2.22	0.40
1:D:220:HIS:HA	1:D:232:VAL:HG12	2.03	0.40
1:A:165:ILE:CD1	1:A:176:LEU:HB2	2.51	0.40
1:C:103:PRO:O	1:C:104:TRP:C	2.64	0.40
1:C:364:TYR:HA	1:C:367:ASP:OD1	2.22	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	416/438 (95%)	406 (98%)	9 (2%)	1 (0%)	43	55
1	B	416/438 (95%)	403 (97%)	11 (3%)	2 (0%)	24	31
1	C	418/438 (95%)	409 (98%)	8 (2%)	1 (0%)	43	55
1	D	418/438 (95%)	404 (97%)	12 (3%)	2 (0%)	24	31
All	All	1668/1752 (95%)	1622 (97%)	40 (2%)	6 (0%)	30	38

All (6) 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	D	317	VAL
1	B	283	ASN

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	328/341 (96%)	323 (98%)	5 (2%)	57	75
1	B	328/341 (96%)	324 (99%)	4 (1%)	63	79
1	C	330/341 (97%)	323 (98%)	7 (2%)	47	66
1	D	330/341 (97%)	323 (98%)	7 (2%)	47	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1316/1364 (96%)	1293 (98%)	23 (2%)	53 72

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	ILE
1	A	252	LEU
1	A	318	LYS
1	A	336	ILE
1	A	388	ILE
1	B	54	VAL
1	B	110	LYS
1	B	371	LEU
1	B	374	THR
1	C	99	SER
1	C	180	ILE
1	C	252	LEU
1	C	318	LYS
1	C	371	LEU
1	C	374	THR
1	C	388	ILE
1	D	54	VAL
1	D	165	ILE
1	D	210	LEU
1	D	238	ASN
1	D	283	ASN
1	D	374	THR
1	D	388	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	90	GLN
1	A	101	HIS
1	A	150	ASN
1	A	160	HIS
1	A	189	GLN
1	A	243	GLN
1	A	258	HIS
1	A	324	HIS

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Mol	Chain	Res	Type
1	A	344	ASN
1	A	352	GLN
1	B	8	GLN
1	B	15	ASN
1	B	97	ASN
1	B	101	HIS
1	B	150	ASN
1	B	160	HIS
1	B	189	GLN
1	B	258	HIS
1	B	321	HIS
1	B	344	ASN
1	B	352	GLN
1	C	90	GLN
1	C	150	ASN
1	C	160	HIS
1	C	189	GLN
1	C	243	GLN
1	C	344	ASN
1	D	90	GLN
1	D	97	ASN
1	D	150	ASN
1	D	160	HIS
1	D	189	GLN
1	D	238	ASN
1	D	243	GLN
1	D	250	GLN
1	D	283	ASN
1	D	344	ASN
1	D	352	GLN
1	D	368	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 [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	418/438 (95%)	-0.15	5 (1%) 76 77	16, 30, 50, 64	0
1	B	418/438 (95%)	-0.12	2 (0%) 87 87	18, 30, 50, 62	0
1	C	420/438 (95%)	-0.46	2 (0%) 87 87	16, 23, 36, 45	0
1	D	420/438 (95%)	-0.31	4 (0%) 79 80	18, 27, 40, 61	0
All	All	1676/1752 (95%)	-0.26	13 (0%) 82 83	16, 27, 45, 64	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	421	ALA	5.2
1	D	316	GLY	4.3
1	B	280	PHE	4.2
1	B	421	ALA	3.7
1	D	106	LYS	2.5
1	A	78	ILE	2.4
1	D	317	VAL	2.4
1	A	4	PHE	2.3
1	D	318	LYS	2.2
1	C	423	VAL	2.2
1	A	420	PRO	2.1
1	C	421	ALA	2.1
1	A	326	ILE	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](#)

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($\text{\AA}^2$)	Q<0.9
2	ZN	D	508	1/1	0.83	0.17	57,57,57,57	1
2	ZN	C	506	1/1	0.84	0.11	51,51,51,51	1
2	ZN	A	502	1/1	0.88	0.10	46,46,46,46	1
2	ZN	B	504	1/1	0.89	0.17	51,51,51,51	1
2	ZN	C	505	1/1	0.97	0.08	58,58,58,58	0
2	ZN	A	501	1/1	0.98	0.06	61,61,61,61	0
2	ZN	D	507	1/1	0.98	0.13	66,66,66,66	0
2	ZN	B	503	1/1	0.98	0.09	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.