



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:28 AM UTC

PDB ID : 2HCV / pdb_00002hcv
Title : Crystal structure of L-rhamnose isomerase from *Pseudomonas stutzeri* with metal ion
Authors : Yoshida, H.; Yamada, M.; Takada, G.; Izumori, K.; Kamitori, S.
Deposited on : 2006-06-19
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

<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

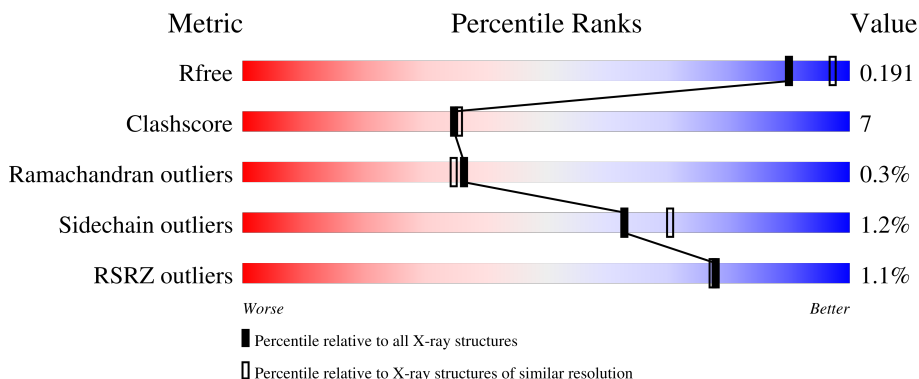
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

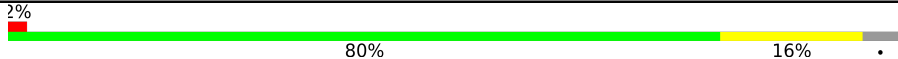
The reported resolution of this entry is 2.00 Å.

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	
1	B	438	
1	C	438	
1	D	438	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14801 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	584	619	9			
1	B	420	Total	C	N	O	S	0	0	0
			3253	2043	583	618	9			
1	C	421	Total	C	N	O	S	0	0	0
			3260	2048	584	619	9			
1	D	417	Total	C	N	O	S	0	0	0
			3237	2034	580	614	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	-	cloning artifact	UNP Q75WH8
A	432	SER	-	cloning artifact	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	-	cloning artifact	UNP Q75WH8
B	432	SER	-	cloning artifact	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	-	cloning artifact	UNP Q75WH8
C	432	SER	-	cloning artifact	UNP Q75WH8

Continued on next page...

Continued from previous page...

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	-	cloning artifact	UNP Q75WH8
D	432	SER	-	cloning artifact	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

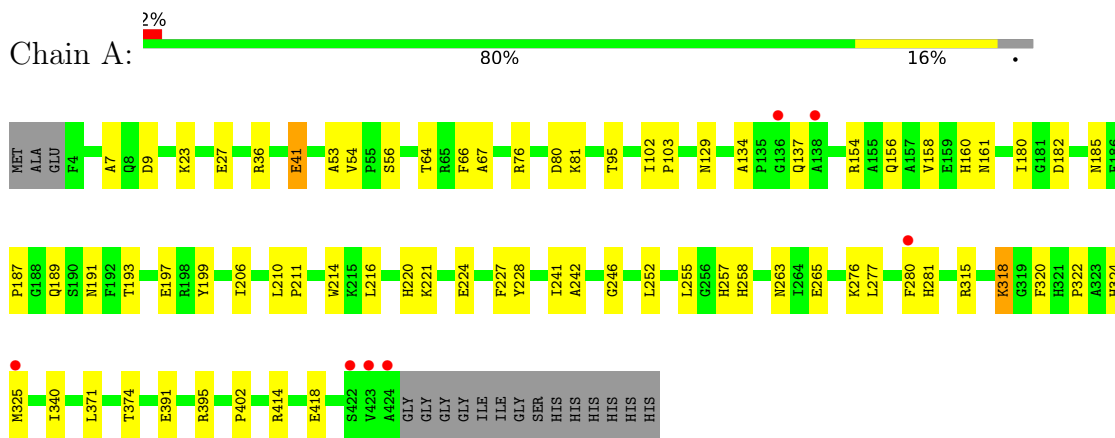
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	408	Total O 408 408	0	0
3	B	474	Total O 474 474	0	0
3	C	420	Total O 420 420	0	0
3	D	481	Total O 481 481	0	0

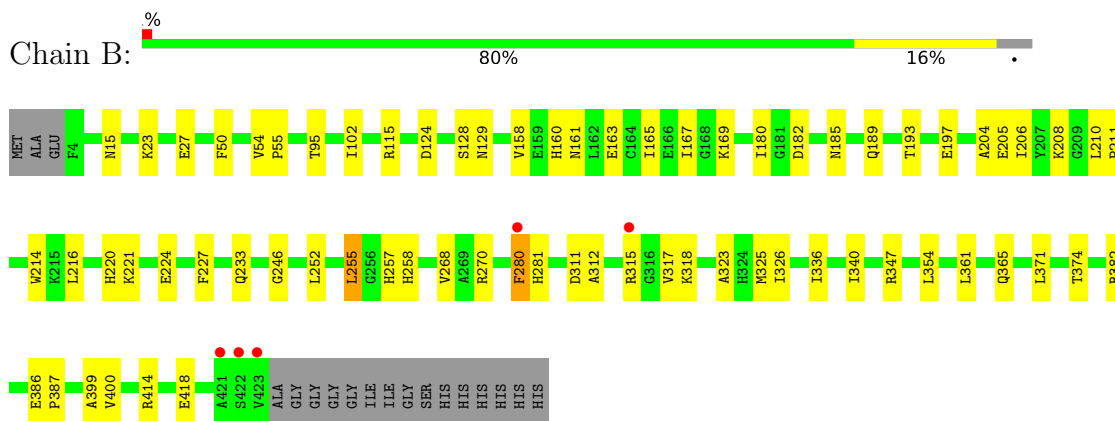
3 Residue-property plots

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.

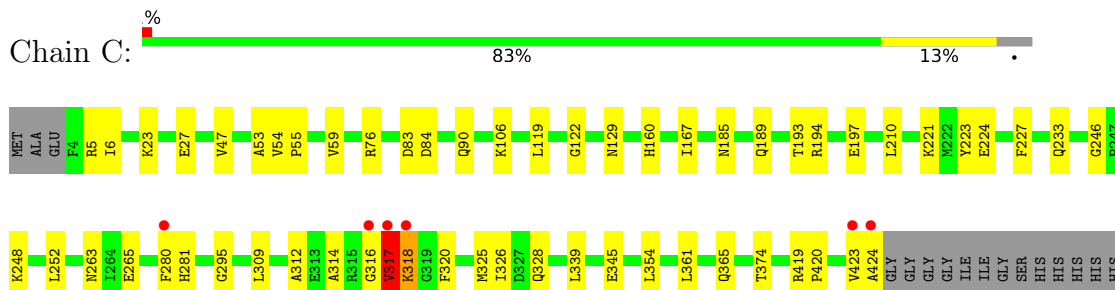
- Molecule 1: L-rhamnose isomerase



- Molecule 1: L-rhamnose isomerase



- Molecule 1: L-rhamnose isomerase



HIS

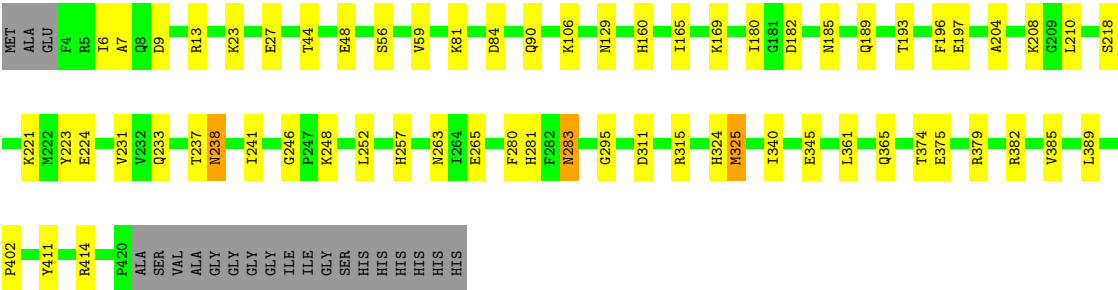
● Molecule 1: L-rhamnose isomerase

Chain D:

81%

14%

5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.26Å 103.97Å 107.02Å 90.00° 106.81° 90.00°	Depositor
Resolution (Å)	48.79 – 2.00 48.79 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.3 (48.79-2.00) 92.3 (48.79-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.25 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.155 , 0.192 0.155 , 0.191	Depositor DCC
R_{free} test set	9706 reflections (9.72%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.8	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	0.96	EDS
Total number of atoms	14801	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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	0.35	0/3332	0.81	4/4518 (0.1%)
1	B	0.35	0/3325	0.83	5/4508 (0.1%)
1	C	0.35	0/3332	0.81	4/4518 (0.1%)
1	D	0.35	0/3309	0.82	3/4486 (0.1%)
All	All	0.35	0/13298	0.82	16/18030 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	GLY	CA-C-N	6.39	126.61	119.32
1	B	246	GLY	C-N-CA	6.39	126.61	119.32
1	A	191	ASN	N-CA-C	-5.86	98.97	108.41
1	A	227	PHE	N-CA-C	5.75	120.30	112.88
1	B	227	PHE	N-CA-C	5.75	119.99	112.92
1	B	255	LEU	N-CA-C	5.60	118.11	111.33
1	C	246	GLY	CA-C-N	5.57	125.93	119.47
1	C	246	GLY	C-N-CA	5.57	125.93	119.47
1	C	122	GLY	N-CA-C	-5.22	105.61	112.81
1	A	246	GLY	CA-C-N	5.20	125.50	119.47
1	A	246	GLY	C-N-CA	5.20	125.50	119.47
1	D	233	GLN	N-CA-C	5.18	118.06	111.69
1	C	227	PHE	N-CA-C	5.14	119.52	112.88
1	B	233	GLN	N-CA-C	5.04	118.57	112.23
1	D	246	GLY	CA-C-N	5.03	124.82	119.28
1	D	246	GLY	C-N-CA	5.03	124.82	119.28

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	52	0
1	B	3253	0	3153	55	0
1	C	3260	0	3165	47	0
1	D	3237	0	3141	40	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	408	0	0	2	0
3	B	474	0	0	14	0
3	C	420	0	0	10	0
3	D	481	0	0	7	0
All	All	14801	0	12624	192	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 7.

All (192) 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	1.13	0.93
1:B:129:ASN:H	1:B:160:HIS:HE1	1.16	0.93
1:C:129:ASN:H	1:C:160:HIS:HE1	1.21	0.88
1:B:128:SER:HA	3:B:886:HOH:O	1.73	0.87
3:B:892:HOH:O	1:D:231:VAL:HG13	1.71	0.87
1:C:47:VAL:HG23	3:C:852:HOH:O	1.79	0.82
1:D:324:HIS:HA	3:D:905:HOH:O	1.80	0.81
1:C:83:ASP:HA	3:C:816:HOH:O	1.82	0.79
1:B:129:ASN:H	1:B:160:HIS:CE1	2.00	0.78
1:A:318:LYS:HA	1:A:318:LYS:HE3	1.64	0.78
1:D:129:ASN:H	1:D:160:HIS:HE1	1.31	0.78
1:C:129:ASN:H	1:C:160:HIS:CE1	2.01	0.78
1:C:210:LEU:HD23	1:C:248:LYS:HE2	1.66	0.77
1:D:129:ASN:H	1:D:160:HIS:CE1	2.03	0.77
1:B:205:GLU:HA	1:B:208:LYS:HE2	1.68	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LEU:HG	1:A:280:PHE:CE1	2.21	0.74
1:C:317:VAL:CG2	1:C:317:VAL:O	2.36	0.74
1:C:354:LEU:HD12	3:C:852:HOH:O	1.87	0.74
1:D:6:ILE:H	1:D:90:GLN:HE22	1.35	0.73
1:B:102:ILE:HB	3:B:886:HOH:O	1.86	0.73
1:A:129:ASN:H	1:A:160:HIS:CE1	2.01	0.73
1:D:280:PHE:HB2	3:D:905:HOH:O	1.88	0.73
1:C:317:VAL:HG23	1:C:320:PHE:HB2	1.71	0.73
1:A:76:ARG:HG2	1:A:80:ASP:OD2	1.89	0.72
1:B:315:ARG:HH12	1:D:193:THR:HB	1.55	0.71
1:C:317:VAL:O	1:C:317:VAL:HG22	1.91	0.71
1:B:158:VAL:HA	1:B:206:ILE:HD11	1.75	0.69
1:C:6:ILE:H	1:C:90:GLN:HE22	1.38	0.69
1:C:5:ARG:HD3	3:C:816:HOH:O	1.94	0.68
1:B:23:LYS:HE2	3:B:813:HOH:O	1.92	0.68
1:A:158:VAL:HA	1:A:206:ILE:HD11	1.77	0.66
1:D:185:ASN:H	1:D:189:GLN:HE22	1.43	0.66
1:C:317:VAL:CG2	1:C:320:PHE:HB2	2.27	0.65
1:D:185:ASN:H	1:D:189:GLN:NE2	1.96	0.64
1:C:23:LYS:O	1:C:27:GLU:HG3	1.97	0.63
1:C:280:PHE:CE2	1:C:309:LEU:HD21	2.33	0.63
1:C:312:ALA:O	1:C:317:VAL:HG13	1.99	0.62
1:B:347:ARG:NH2	3:B:873:HOH:O	2.31	0.61
1:B:280:PHE:HB3	3:B:899:HOH:O	2.01	0.61
1:D:210:LEU:HD23	1:D:248:LYS:HE2	1.83	0.60
1:C:53:ALA:HB3	1:C:325:MET:HG2	1.83	0.60
1:B:311:ASP:O	1:B:315:ARG:HG2	2.02	0.60
1:C:119:LEU:HD22	3:C:816:HOH:O	2.02	0.60
1:A:255:LEU:HG	1:A:280:PHE:HE1	1.63	0.59
1:B:315:ARG:HG3	1:B:317:VAL:HG23	1.83	0.58
1:B:220:HIS:HE2	1:B:258:HIS:CE1	2.21	0.58
1:C:76:ARG:NH1	1:C:419:ARG:HG2	2.18	0.58
1:D:44:THR:O	1:D:48:GLU:HG2	2.04	0.58
3:B:892:HOH:O	1:D:196:PHE:HB2	2.04	0.58
1:A:41:GLU:OE2	1:A:395:ARG:NH2	2.30	0.57
1:D:7:ALA:HB1	1:D:9:ASP:OD1	2.03	0.57
1:D:23:LYS:O	1:D:27:GLU:HG3	2.05	0.57
1:D:193:THR:O	1:D:197:GLU:HG3	2.05	0.57
1:B:15:ASN:ND2	1:B:400:VAL:H	2.02	0.56
1:C:328:GLN:NE2	3:C:838:HOH:O	2.37	0.56
1:A:54:VAL:HG13	1:A:95:THR:HB	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLN:HG2	1:A:156:GLN:HE22	1.70	0.56
1:B:15:ASN:HD21	1:B:400:VAL:H	1.54	0.56
1:B:185:ASN:H	1:B:189:GLN:HE22	1.54	0.56
1:B:23:LYS:O	1:B:27:GLU:HG3	2.07	0.55
1:C:185:ASN:H	1:C:189:GLN:HE22	1.53	0.55
1:A:185:ASN:H	1:A:189:GLN:HE22	1.54	0.55
1:A:220:HIS:HE2	1:A:258:HIS:CE1	2.25	0.55
1:A:252:LEU:HD21	1:A:281:HIS:CG	2.42	0.55
1:B:185:ASN:H	1:B:189:GLN:NE2	2.05	0.55
1:D:180:ILE:HD12	1:D:182:ASP:CG	2.32	0.55
1:B:50:PHE:N	3:B:873:HOH:O	2.40	0.54
1:B:180:ILE:HD12	1:B:182:ASP:CG	2.33	0.54
1:C:106:LYS:HE2	1:C:167:ILE:HD11	1.88	0.54
1:A:391:GLU:O	1:A:395:ARG:HG3	2.07	0.54
1:B:365:GLN:HG2	3:D:884:HOH:O	2.07	0.54
1:B:193:THR:O	1:B:197:GLU:HG3	2.06	0.54
1:B:210:LEU:HD11	1:B:216:LEU:HB2	1.90	0.53
1:B:414:ARG:O	1:B:418:GLU:HG3	2.08	0.53
1:B:270:ARG:NH2	3:B:892:HOH:O	2.40	0.53
1:C:193:THR:O	1:C:197:GLU:HG3	2.09	0.53
1:C:76:ARG:HH12	1:C:419:ARG:HG2	1.73	0.53
1:A:263:ASN:OD1	1:A:265:GLU:HG2	2.10	0.52
1:C:59:VAL:HG11	1:C:84:ASP:HB2	1.91	0.52
1:B:365:GLN:HA	3:D:884:HOH:O	2.10	0.52
1:C:185:ASN:H	1:C:189:GLN:NE2	2.08	0.52
1:C:280:PHE:HE2	1:C:309:LEU:HD21	1.74	0.52
1:D:325:MET:HE2	3:D:546:HOH:O	2.10	0.52
1:A:158:VAL:HG13	1:A:206:ILE:HD13	1.91	0.51
1:A:324:HIS:C	1:A:325:MET:HG3	2.35	0.51
1:A:161:ASN:HB2	1:A:206:ILE:HD12	1.92	0.51
1:B:158:VAL:HG13	1:B:206:ILE:HD13	1.91	0.51
1:A:220:HIS:HE2	1:A:258:HIS:HE1	1.58	0.51
1:D:263:ASN:OD1	1:D:265:GLU:HG2	2.11	0.51
1:A:185:ASN:H	1:A:189:GLN:NE2	2.09	0.51
1:C:252:LEU:HD21	1:C:281:HIS:CG	2.46	0.51
1:A:53:ALA:HB3	1:A:325:MET:HG2	1.93	0.50
1:C:263:ASN:OD1	1:C:265:GLU:HG2	2.11	0.50
1:C:317:VAL:CG2	1:C:320:PHE:CB	2.89	0.50
1:A:255:LEU:HG	1:A:280:PHE:CZ	2.47	0.50
1:A:193:THR:O	1:A:197:GLU:HG3	2.12	0.50
1:D:361:LEU:O	1:D:365:GLN:HG3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ARG:HH12	1:D:193:THR:CB	2.25	0.49
1:A:414:ARG:O	1:A:418:GLU:HG3	2.11	0.48
1:B:252:LEU:HD21	1:B:281:HIS:CG	2.48	0.48
1:A:242:ALA:HB1	1:A:276:LYS:HD2	1.95	0.48
1:C:221:LYS:HE2	1:C:223:TYR:O	2.12	0.48
1:A:180:ILE:HD12	1:A:182:ASP:CG	2.39	0.48
1:A:129:ASN:N	1:A:160:HIS:HE1	1.96	0.48
1:B:280:PHE:O	1:B:325:MET:HE3	2.14	0.48
1:B:323:ALA:C	1:B:325:MET:HE2	2.39	0.48
1:D:311:ASP:OD2	1:D:315:ARG:HD3	2.13	0.48
1:B:15:ASN:HD21	1:B:399:ALA:HA	1.79	0.47
1:B:115:ARG:HD3	3:B:877:HOH:O	2.13	0.47
1:D:283:ASN:C	1:D:283:ASN:HD22	2.22	0.47
1:B:163:GLU:O	1:B:167:ILE:HG12	2.13	0.47
1:B:165:ILE:O	1:B:169:LYS:HG3	2.14	0.47
1:B:268:VAL:CG2	1:B:280:PHE:HZ	2.27	0.47
1:D:252:LEU:HD21	1:D:281:HIS:CG	2.48	0.47
1:C:55:PRO:HD3	1:C:326:ILE:O	2.14	0.47
1:B:161:ASN:HB2	1:B:206:ILE:HD12	1.95	0.47
1:B:221:LYS:HA	1:B:257:HIS:HB3	1.96	0.47
1:B:220:HIS:HE2	1:B:258:HIS:HE1	1.62	0.46
3:A:729:HOH:O	1:D:382:ARG:HD3	2.15	0.46
1:B:312:ALA:HA	1:B:315:ARG:HE	1.81	0.46
1:D:221:LYS:HA	1:D:257:HIS:HB3	1.98	0.46
1:A:137:GLN:HG2	1:A:156:GLN:NE2	2.29	0.46
1:A:210:LEU:HD11	1:A:216:LEU:HB2	1.97	0.46
1:A:211:PRO:HD2	1:A:214:TRP:CG	2.50	0.46
1:B:54:VAL:HG13	1:B:95:THR:HB	1.98	0.45
1:D:237:THR:O	1:D:241:ILE:HG13	2.16	0.45
1:C:312:ALA:O	1:C:317:VAL:CG1	2.64	0.45
1:A:315:ARG:NH2	3:C:628:HOH:O	2.50	0.45
1:B:361:LEU:O	1:B:365:GLN:HG3	2.16	0.45
1:A:154:ARG:O	1:A:158:VAL:HG23	2.16	0.45
1:A:7:ALA:HB1	1:A:9:ASP:OD1	2.18	0.44
1:A:187:PRO:HA	1:A:228:TYR:CE2	2.53	0.44
1:D:13:ARG:HH11	1:D:13:ARG:HG3	1.82	0.44
1:C:318:LYS:H	1:C:318:LYS:HG3	1.49	0.44
1:B:129:ASN:N	1:B:160:HIS:HE1	1.99	0.44
1:C:54:VAL:HG11	3:C:843:HOH:O	2.17	0.44
1:A:161:ASN:HB2	1:A:206:ILE:CD1	2.47	0.44
1:C:423:VAL:HG12	1:C:424:ALA:N	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:LEU:O	1:C:365:GLN:HG3	2.18	0.44
1:A:221:LYS:HA	1:A:257:HIS:HB3	1.99	0.43
1:B:211:PRO:HD2	1:B:214:TRP:CG	2.52	0.43
1:C:129:ASN:N	1:C:160:HIS:HE1	2.03	0.43
1:B:382:ARG:HD3	3:B:685:HOH:O	2.17	0.43
1:C:194:ARG:HD3	1:C:197:GLU:OE1	2.18	0.43
1:D:411:TYR:O	1:D:414:ARG:HB3	2.19	0.43
1:A:23:LYS:O	1:A:27:GLU:HG3	2.18	0.43
1:C:76:ARG:HH11	1:C:76:ARG:HG3	1.83	0.43
1:C:339:LEU:HA	3:C:838:HOH:O	2.18	0.43
1:A:134:ALA:O	1:A:137:GLN:HB2	2.19	0.42
1:D:165:ILE:HG22	1:D:169:LYS:HD2	2.00	0.42
1:A:161:ASN:CB	1:A:206:ILE:HD12	2.49	0.42
1:A:340:ILE:HG21	1:A:402:PRO:HB2	2.01	0.42
1:B:204:ALA:O	1:B:208:LYS:HG3	2.20	0.42
1:C:76:ARG:HD3	1:C:420:PRO:CD	2.49	0.42
1:D:340:ILE:HG21	1:D:402:PRO:HB2	2.01	0.42
1:A:56:SER:O	1:A:81:LYS:HD3	2.19	0.42
1:B:255:LEU:HD21	1:B:280:PHE:CE1	2.55	0.42
1:B:268:VAL:CG2	1:B:280:PHE:CZ	3.02	0.42
1:C:354:LEU:CD1	3:C:852:HOH:O	2.56	0.42
1:D:295:GLY:HA3	1:D:345:GLU:HG2	2.02	0.42
1:B:318:LYS:HG3	3:B:917:HOH:O	2.20	0.42
1:D:59:VAL:HG11	1:D:84:ASP:HB2	2.02	0.42
1:D:218:SER:OG	1:D:238:ASN:ND2	2.52	0.42
1:A:137:GLN:CG	1:A:156:GLN:NE2	2.83	0.41
1:D:385:VAL:O	1:D:389:LEU:HD13	2.19	0.41
1:B:281:HIS:C	3:B:899:HOH:O	2.64	0.41
1:A:66:PHE:O	1:A:67:ALA:HB2	2.19	0.41
1:C:295:GLY:HA3	1:C:345:GLU:HG2	2.01	0.41
1:A:252:LEU:HD21	1:A:281:HIS:CD2	2.56	0.41
1:A:277:LEU:C	1:A:277:LEU:HD13	2.45	0.41
1:D:106:LYS:HA	3:D:979:HOH:O	2.20	0.41
1:A:158:VAL:HG13	1:A:206:ILE:CD1	2.50	0.41
1:A:36:ARG:HG2	3:A:638:HOH:O	2.21	0.41
1:C:314:ALA:C	1:C:316:GLY:H	2.29	0.41
1:D:221:LYS:HE2	1:D:223:TYR:O	2.21	0.41
1:C:252:LEU:HD23	1:C:252:LEU:C	2.46	0.41
1:D:375:GLU:O	1:D:379:ARG:HG3	2.21	0.41
1:B:55:PRO:HD3	1:B:326:ILE:O	2.20	0.40
1:B:336:ILE:O	1:B:340:ILE:HG13	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:VAL:CG1	1:C:424:ALA:N	2.83	0.40
1:A:102:ILE:CG2	1:A:103:PRO:HA	2.52	0.40
1:A:320:PHE:CE1	1:A:322:PRO:HD3	2.57	0.40
1:A:64:THR:HB	3:B:613:HOH:O	2.22	0.40
1:A:199:TYR:CE1	1:A:241:ILE:HD13	2.56	0.40
1:B:386:GLU:HB3	1:B:387:PRO:HD3	2.03	0.40
1:C:221:LYS:O	1:C:233:GLN:HA	2.22	0.40
1:D:204:ALA:O	1:D:208:LYS:HG3	2.21	0.40
1:B:268:VAL:HG22	1:B:280:PHE:CZ	2.56	0.40
1:D:160:HIS:HD2	3:D:723:HOH:O	2.05	0.40
1:A:102:ILE:HG23	1:A:103:PRO:HA	2.04	0.40
1:B:268:VAL:HG21	1:B:280:PHE:HZ	1.86	0.40
1:D:56:SER:O	1:D:81:LYS:HD3	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	419/438 (96%)	410 (98%)	8 (2%)	1 (0%)	43	42
1	B	418/438 (95%)	407 (97%)	10 (2%)	1 (0%)	43	42
1	C	419/438 (96%)	404 (96%)	13 (3%)	2 (0%)	24	21
1	D	415/438 (95%)	404 (97%)	10 (2%)	1 (0%)	43	42
All	All	1671/1752 (95%)	1625 (97%)	41 (2%)	5 (0%)	36	35

All (5) Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	224	GLU
1	C	224	GLU
1	D	224	GLU

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%)	326 (99%)	4 (1%)	63	70
1	B	329/341 (96%)	324 (98%)	5 (2%)	57	64
1	C	330/341 (97%)	327 (99%)	3 (1%)	70	78
1	D	328/341 (96%)	324 (99%)	4 (1%)	63	70
All	All	1317/1364 (97%)	1301 (99%)	16 (1%)	63	70

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

Mol	Chain	Res	Type
1	A	41	GLU
1	A	318	LYS
1	A	371	LEU
1	A	374	THR
1	B	124	ASP
1	B	280	PHE
1	B	354	LEU
1	B	371	LEU
1	B	374	THR
1	C	317	VAL
1	C	318	LYS
1	C	374	THR
1	D	238	ASN
1	D	283	ASN
1	D	325	MET
1	D	374	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	97	ASN
1	A	160	HIS
1	A	189	GLN
1	A	250	GLN
1	A	258	HIS
1	A	321	HIS
1	A	328	GLN
1	A	344	ASN
1	A	352	GLN
1	B	8	GLN
1	B	15	ASN
1	B	127	ASN
1	B	150	ASN
1	B	160	HIS
1	B	189	GLN
1	B	250	GLN
1	B	258	HIS
1	B	344	ASN
1	C	8	GLN
1	C	90	GLN
1	C	139	HIS
1	C	160	HIS
1	C	189	GLN
1	C	243	GLN
1	C	328	GLN
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	283	ASN
1	D	321	HIS
1	D	344	ASN
1	D	352	GLN
1	D	365	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 [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](#)

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

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	421/438 (96%)	-0.37	7 (1%) 69 68	12, 18, 32, 53	0
1	B	420/438 (95%)	-0.48	5 (1%) 76 76	10, 16, 29, 50	0
1	C	421/438 (96%)	-0.36	6 (1%) 73 73	12, 18, 35, 60	0
1	D	417/438 (95%)	-0.52	0 100 100	11, 17, 27, 38	0
All	All	1679/1752 (95%)	-0.43	18 (1%) 78 77	10, 17, 31, 60	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	424	ALA	4.4
1	B	423	VAL	4.2
1	A	424	ALA	3.9
1	A	280	PHE	3.9
1	C	317	VAL	3.5
1	A	136	GLY	3.4
1	C	316	GLY	3.2
1	A	422	SER	3.0
1	B	280	PHE	3.0
1	A	138	ALA	2.9
1	A	423	VAL	2.9
1	C	423	VAL	2.8
1	C	318	LYS	2.8
1	B	421	ALA	2.7
1	C	280	PHE	2.3
1	B	422	SER	2.2
1	A	325	MET	2.2
1	B	315	ARG	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 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	C	506	1/1	0.90	0.08	57,57,57,57	1
2	ZN	B	504	1/1	0.92	0.06	50,50,50,50	1
2	ZN	A	502	1/1	0.93	0.08	54,54,54,54	1
2	ZN	D	508	1/1	0.95	0.07	40,40,40,40	1
2	ZN	B	503	1/1	0.99	0.05	30,30,30,30	0
2	ZN	D	507	1/1	0.99	0.03	26,26,26,26	0
2	ZN	A	501	1/1	0.99	0.06	32,32,32,32	0
2	ZN	C	505	1/1	1.00	0.06	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.