



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 05:46 PM EDT

PDB ID : 4R1O
Title : Crystal Structure of Thermophilic Geobacillus kaustophilus L-Arabinose isomerase
Authors : Choi, J.M.; Lee, Y.J.; Lee, D.W.; Lee, S.H.
Deposited on : 2014-08-07
Resolution : 2.40 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

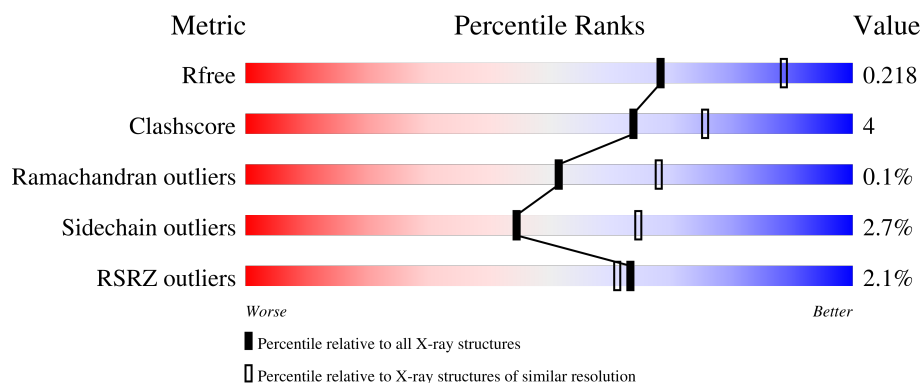
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	497	<div> <div>90%</div> <div>10%</div> </div>
1	B	497	<div> <div>2%</div> <div>89%</div> <div>11%</div> </div>
1	C	497	<div> <div>2%</div> <div>88%</div> <div>11%</div> </div>
1	D	497	<div> <div>2%</div> <div>87%</div> <div>12%</div> </div>
1	E	497	<div> <div>5%</div> <div>84%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	497	<div><div></div><div>4%87%12%..</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24843 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-arabinose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3953	2514	693	724	22			
1	B	495	Total	C	N	O	S	0	0	0
			3942	2508	689	723	22			
1	C	496	Total	C	N	O	S	0	0	0
			3953	2514	693	724	22			
1	D	496	Total	C	N	O	S	0	0	0
			3953	2514	693	724	22			
1	E	494	Total	C	N	O	S	0	0	0
			3934	2503	688	722	21			
1	F	493	Total	C	N	O	S	0	0	0
			3926	2497	687	721	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	SEE REMARK 999	UNP Q5KYP7
B	1	MET	-	SEE REMARK 999	UNP Q5KYP7
C	1	MET	-	SEE REMARK 999	UNP Q5KYP7
D	1	MET	-	SEE REMARK 999	UNP Q5KYP7
E	1	MET	-	SEE REMARK 999	UNP Q5KYP7
F	1	MET	-	SEE REMARK 999	UNP Q5KYP7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	230	Total	O	0	0
			230	230		
2	B	213	Total	O	0	0
			213	213		
2	C	220	Total	O	0	0
			220	220		

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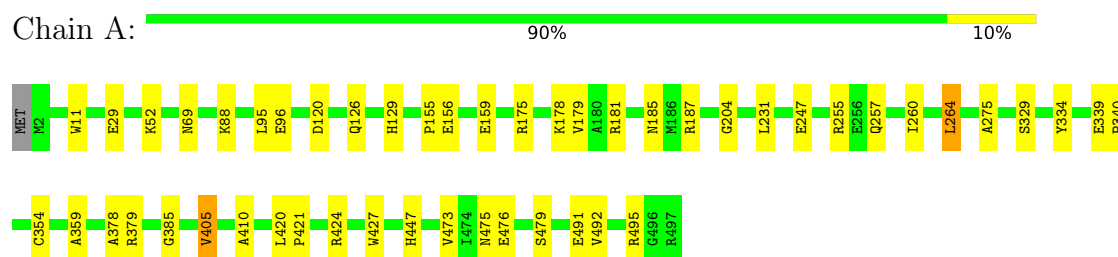
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	191	Total 191	O 191	0	0
2	E	160	Total 160	O 160	0	0
2	F	168	Total 168	O 168	0	0

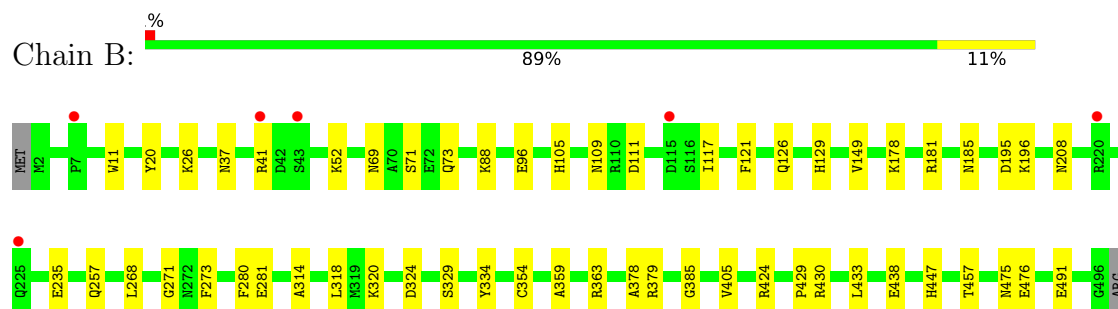
3 Residue-property plots

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.

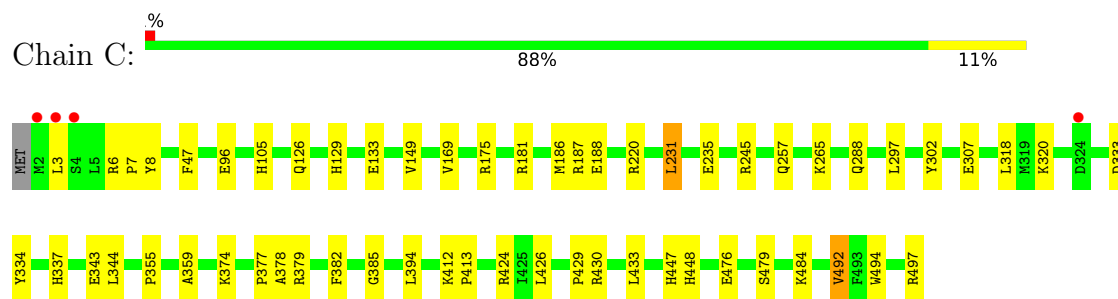
- Molecule 1: L-arabinose isomerase



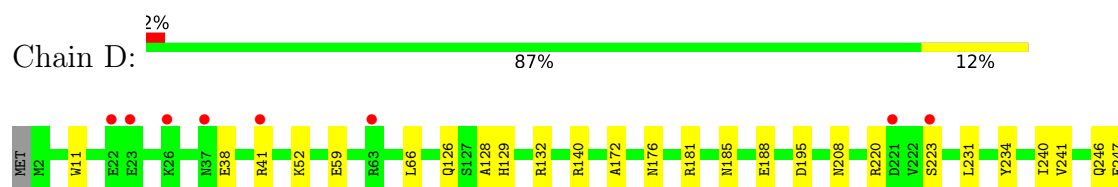
- Molecule 1: L-arabinose isomerase

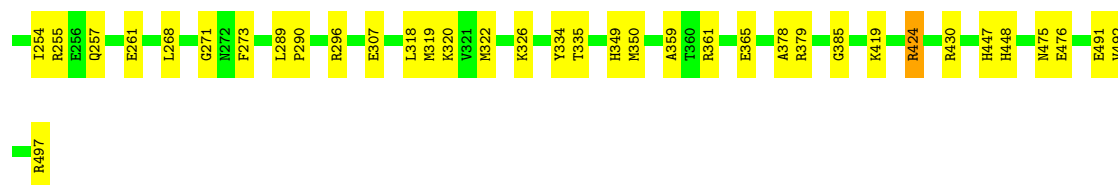


- Molecule 1: L-arabinose isomerase

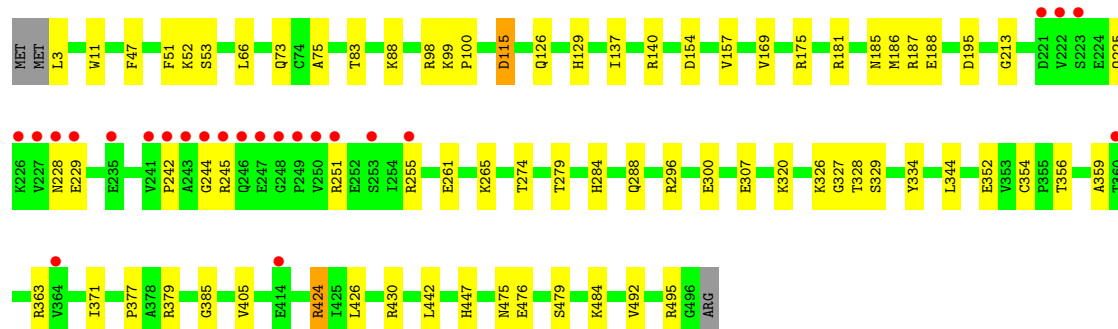
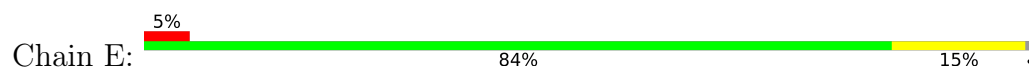


- Molecule 1: L-arabinose isomerase

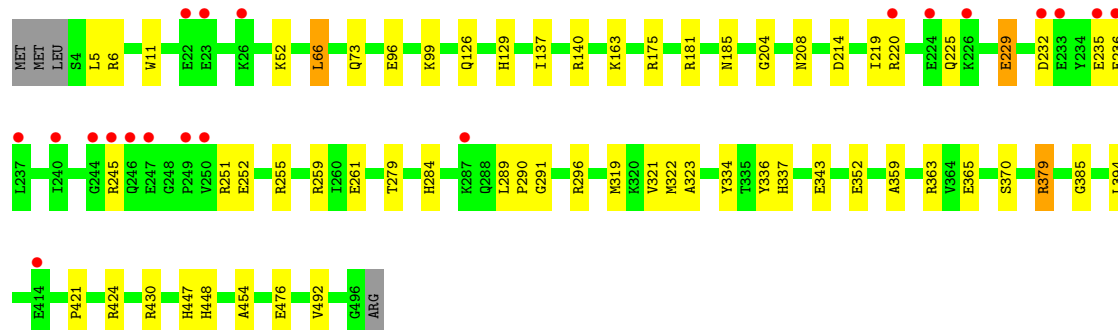
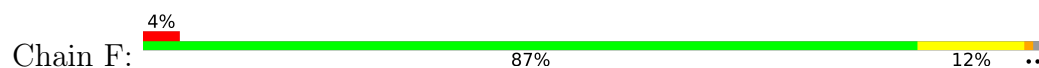




- Molecule 1: L-arabinose isomerase



- Molecule 1: L-arabinose isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.72Å 140.75Å 215.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.32 – 2.40 48.23 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.8 (45.32-2.40) 94.9 (48.23-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.66 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.164 , 0.216 0.167 , 0.218	Depositor DCC
R_{free} test set	6608 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24843	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.41	0/4052	0.55	0/5486
1	B	0.40	0/4041	0.55	0/5472
1	C	0.41	0/4052	0.55	0/5486
1	D	0.39	0/4052	0.54	0/5486
1	E	0.38	0/4033	0.53	0/5462
1	F	0.38	0/4025	0.55	0/5451
All	All	0.39	0/24255	0.54	0/32843

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	3953	0	3846	32	0
1	B	3942	0	3833	33	0
1	C	3953	0	3846	32	0
1	D	3953	0	3846	43	0
1	E	3934	0	3824	46	0
1	F	3926	0	3813	38	0
2	A	230	0	0	3	0
2	B	213	0	0	5	0
2	C	220	0	0	5	0
2	D	191	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	160	0	0	1	0
2	F	168	0	0	3	0
All	All	24843	0	23008	197	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 4.

All (197) 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:F:6:ARG:HH21	1:F:73:GLN:HG3	1.39	0.85
1:F:430:ARG:HD3	1:F:476:GLU:HG3	1.62	0.80
1:C:447:HIS:HB2	1:E:129:HIS:HB2	1.63	0.80
1:B:129:HIS:HB2	1:E:447:HIS:HB2	1.65	0.79
1:D:129:HIS:HB2	1:F:447:HIS:HB2	1.66	0.78
1:B:359:ALA:HB2	1:B:385:GLY:HA2	1.69	0.75
1:A:447:HIS:HB2	1:F:129:HIS:HB2	1.70	0.73
1:E:320:LYS:HD2	1:E:328:THR:HB	1.70	0.72
1:A:29:GLU:OE2	2:A:692:HOH:O	2.08	0.71
1:E:327:GLY:HA2	1:E:356:THR:HG23	1.73	0.70
1:A:126:GLN:HB2	1:A:129:HIS:CE1	2.27	0.70
1:C:448:HIS:NE2	2:C:604:HOH:O	2.25	0.70
1:B:447:HIS:HB2	1:C:129:HIS:HB2	1.74	0.68
1:A:359:ALA:HB2	1:A:385:GLY:HA2	1.75	0.68
1:E:430:ARG:HD3	1:E:476:GLU:HG3	1.75	0.68
1:E:186:MET:HB2	1:E:307:GLU:HB2	1.76	0.67
1:F:448:HIS:NE2	2:F:582:HOH:O	2.29	0.65
1:F:359:ALA:HB2	1:F:385:GLY:HA2	1.78	0.65
1:C:430:ARG:HD3	1:C:476:GLU:HG3	1.79	0.65
1:D:132:ARG:NH1	1:F:336:TYR:OH	2.30	0.65
1:C:3:LEU:HD21	1:C:302:TYR:CZ	2.33	0.64
1:F:66:LEU:HD13	1:F:96:GLU:HG2	1.80	0.64
1:F:252:GLU:OE1	1:F:255:ARG:NH1	2.31	0.64
1:C:359:ALA:HB2	1:C:385:GLY:HA2	1.81	0.63
1:A:491:GLU:OE2	1:A:495:ARG:NH1	2.23	0.62
1:D:359:ALA:HB2	1:D:385:GLY:HA2	1.82	0.62
1:D:430:ARG:HD3	1:D:476:GLU:HG3	1.82	0.61
1:A:247:GLU:OE2	1:A:255:ARG:NH2	2.34	0.61
1:E:442:LEU:HD13	1:E:484:LYS:HG2	1.82	0.61
1:D:172:ALA:O	1:D:176:ASN:ND2	2.33	0.61
1:E:98:ARG:O	1:E:175:ARG:NH2	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:501:HOH:O	1:F:181:ARG:HD3	2.02	0.60
1:B:430:ARG:HD3	1:B:476:GLU:HG3	1.83	0.60
1:D:128:ALA:O	1:D:132:ARG:HD2	2.02	0.59
1:D:448:HIS:NE2	2:D:586:HOH:O	2.31	0.59
1:A:88:LYS:HE3	1:D:188:GLU:HA	1.84	0.59
1:D:231:LEU:HD11	1:D:254:ILE:HG22	1.83	0.59
1:F:261:GLU:OE1	1:F:296:ARG:NH1	2.36	0.58
1:A:129:HIS:HB2	1:D:447:HIS:HB2	1.84	0.58
1:C:181:ARG:HD3	2:D:505:HOH:O	2.05	0.57
1:D:491:GLU:HG2	2:D:674:HOH:O	2.06	0.56
1:F:126:GLN:HB2	1:F:129:HIS:CE1	2.42	0.55
1:C:96:GLU:HG3	2:C:669:HOH:O	2.05	0.55
1:E:181:ARG:HD3	2:F:536:HOH:O	2.04	0.55
1:A:491:GLU:HG2	2:A:708:HOH:O	2.07	0.55
1:B:129:HIS:HB2	1:E:447:HIS:CB	2.37	0.54
1:B:11:TRP:CD2	1:B:52:LYS:HE3	2.42	0.54
1:A:257:GLN:HG3	1:A:378:ALA:HB3	1.89	0.54
1:D:257:GLN:HG3	1:D:378:ALA:HB3	1.89	0.54
1:A:11:TRP:CD2	1:A:52:LYS:HE3	2.42	0.53
1:A:96:GLU:HG3	2:A:717:HOH:O	2.08	0.53
1:E:359:ALA:HB2	1:E:385:GLY:HA2	1.89	0.53
1:D:11:TRP:CD2	1:D:52:LYS:HE3	2.44	0.53
1:D:38:GLU:OE1	1:D:41:ARG:NH2	2.39	0.53
1:F:163:LYS:HE2	2:F:555:HOH:O	2.08	0.53
1:B:88:LYS:HE2	1:E:188:GLU:HA	1.91	0.53
1:D:129:HIS:HB2	1:F:447:HIS:CB	2.38	0.53
1:D:289:LEU:HD12	1:D:290:PRO:HD2	1.91	0.53
1:B:329:SER:HB2	1:B:354:CYS:HB3	1.91	0.52
1:A:447:HIS:H	1:A:447:HIS:CD2	2.27	0.51
1:C:235:GLU:OE2	1:C:245:ARG:NH1	2.44	0.51
1:E:261:GLU:OE1	1:E:296:ARG:HD3	2.10	0.51
1:B:314:ALA:O	1:B:318:LEU:HG	2.11	0.51
1:B:438:GLU:OE1	2:B:570:HOH:O	2.19	0.51
1:F:235:GLU:OE1	1:F:251:ARG:NH1	2.35	0.51
1:B:69:ASN:ND2	1:B:96:GLU:O	2.31	0.51
1:B:447:HIS:CB	1:C:129:HIS:HB2	2.41	0.51
1:B:117:ILE:HG13	1:B:121:PHE:CD1	2.46	0.51
1:B:126:GLN:HB2	1:B:129:HIS:CE1	2.46	0.50
1:E:83:THR:HA	1:E:126:GLN:HG3	1.92	0.50
1:C:320:LYS:HE2	2:C:578:HOH:O	2.10	0.50
2:C:508:HOH:O	1:D:181:ARG:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:LYS:NZ	2:C:714:HOH:O	2.32	0.49
1:B:235:GLU:HB3	2:B:681:HOH:O	2.11	0.49
1:C:265:LYS:HG3	1:C:297:LEU:HD21	1.94	0.49
1:D:307:GLU:OE1	2:D:586:HOH:O	2.19	0.49
1:A:181:ARG:HD3	2:B:503:HOH:O	2.13	0.49
1:E:344:LEU:HD13	1:E:426:LEU:HD22	1.95	0.49
1:E:326:LYS:HG3	1:E:356:THR:OG1	2.12	0.49
1:A:179:VAL:HG22	1:A:275:ALA:HB3	1.94	0.49
1:D:11:TRP:CE3	1:D:52:LYS:HE3	2.48	0.49
1:D:140:ARG:NH2	1:E:195:ASP:OD2	2.46	0.49
1:F:289:LEU:HD12	1:F:290:PRO:HD2	1.95	0.49
1:D:424:ARG:N	1:D:424:ARG:HD3	2.28	0.48
1:D:59:GLU:H	1:D:59:GLU:CD	2.16	0.48
1:C:492:VAL:HG11	1:E:492:VAL:HG12	1.94	0.48
1:E:187:ARG:HG2	1:F:208:ASN:HB3	1.96	0.48
1:B:429:PRO:HG2	1:B:433:LEU:HA	1.96	0.48
1:E:47:PHE:CE2	1:E:169:VAL:HG21	2.48	0.48
1:D:261:GLU:OE1	1:D:296:ARG:HD3	2.13	0.47
1:D:271:GLY:HA3	1:D:273:PHE:CE2	2.49	0.47
1:F:232:ASP:O	1:F:236:GLU:HG2	2.15	0.47
1:A:447:HIS:CB	1:F:129:HIS:HB2	2.40	0.47
1:B:181:ARG:NH2	1:B:185:ASN:OD1	2.48	0.47
1:F:181:ARG:NH2	1:F:185:ASN:OD1	2.48	0.47
1:A:475:ASN:HB2	1:A:476:GLU:OE1	2.15	0.47
1:F:11:TRP:CD2	1:F:52:LYS:HE3	2.50	0.47
1:E:484:LYS:HE2	1:E:484:LYS:HB3	1.82	0.47
1:F:352:GLU:N	1:F:352:GLU:OE1	2.45	0.46
1:E:213:GLY:HA3	1:F:284:HIS:CD2	2.51	0.46
1:A:405:VAL:HG13	1:A:473:VAL:HG22	1.97	0.46
1:F:66:LEU:HD13	1:F:96:GLU:CG	2.44	0.46
1:C:429:PRO:HG2	1:C:433:LEU:HA	1.98	0.46
1:E:181:ARG:NH2	1:E:185:ASN:OD1	2.48	0.46
1:B:37:ASN:HB3	1:B:41:ARG:NH2	2.31	0.46
1:E:75:ALA:O	1:E:100:PRO:HG2	2.16	0.46
1:E:284:HIS:NE2	1:F:214:ASP:OD1	2.37	0.46
1:B:109:ASN:ND2	1:B:111:ASP:O	2.43	0.45
1:E:228:ASN:OD1	1:E:255:ARG:NH2	2.41	0.45
1:E:242:PRO:HA	1:E:245:ARG:HE	1.81	0.45
1:E:329:SER:HB2	1:E:354:CYS:HB3	1.97	0.45
1:E:115:ASP:OD1	1:E:115:ASP:N	2.44	0.45
1:A:187:ARG:HG2	1:B:208:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:TYR:HE2	1:E:371:ILE:HD11	1.81	0.45
1:B:105:HIS:HB3	1:B:149:VAL:HG22	1.98	0.45
1:D:359:ALA:HB2	1:D:385:GLY:CA	2.46	0.45
1:E:11:TRP:CE2	1:E:52:LYS:HE3	2.52	0.45
1:F:99:LYS:HD3	1:F:99:LYS:HA	1.77	0.45
1:B:178:LYS:HE2	1:B:178:LYS:HB3	1.85	0.45
1:F:379:ARG:NH2	1:F:421:PRO:O	2.47	0.45
1:B:491:GLU:HG2	2:B:661:HOH:O	2.16	0.45
1:D:475:ASN:HB2	1:D:476:GLU:OE1	2.17	0.45
1:E:265:LYS:NZ	1:E:300:GLU:OE2	2.50	0.45
1:F:175:ARG:HA	1:F:204:GLY:HA3	1.97	0.45
1:B:37:ASN:HB3	1:B:41:ARG:HH22	1.83	0.44
1:B:257:GLN:HG3	1:B:378:ALA:HB3	1.98	0.44
1:D:126:GLN:HB2	1:D:129:HIS:CE1	2.53	0.44
1:D:320:LYS:HE3	2:D:573:HOH:O	2.16	0.44
1:C:186:MET:HB2	1:C:307:GLU:HB3	1.98	0.44
1:C:344:LEU:HD13	1:C:426:LEU:HD22	2.00	0.44
1:C:6:ARG:HB2	1:C:8:TYR:CE2	2.53	0.44
1:C:188:GLU:O	1:E:88:LYS:HB2	2.18	0.44
1:B:271:GLY:HA3	1:B:273:PHE:CE2	2.53	0.43
1:D:195:ASP:OD2	1:E:140:ARG:NH2	2.51	0.43
1:D:320:LYS:HZ1	1:D:326:LYS:HE3	1.83	0.43
1:C:126:GLN:HB2	1:C:129:HIS:CE1	2.53	0.43
1:A:155:PRO:O	1:A:159:GLU:HG2	2.18	0.43
1:E:288:GLN:OE1	1:E:377:PRO:HA	2.18	0.43
1:F:323:ALA:HB1	1:F:454:ALA:HB3	2.01	0.43
1:B:280:PHE:CE1	1:B:281:GLU:HG3	2.54	0.43
1:F:363:ARG:HG2	1:F:365:GLU:HG2	2.00	0.43
1:A:260:ILE:O	1:A:264:LEU:HB2	2.18	0.43
1:B:475:ASN:HB2	1:B:476:GLU:OE1	2.18	0.43
1:C:257:GLN:HG3	1:C:378:ALA:HB3	1.99	0.43
1:C:3:LEU:HD22	1:C:3:LEU:N	2.34	0.43
1:F:319:MET:HA	1:F:322:MET:HG2	1.99	0.42
1:A:420:LEU:HD12	1:A:421:PRO:HD2	2.01	0.42
1:C:105:HIS:HB3	1:C:149:VAL:HG22	2.01	0.42
1:F:137:ILE:HD12	1:F:137:ILE:HA	1.80	0.42
1:C:187:ARG:HG2	1:D:208:ASN:HB3	2.00	0.42
1:D:234:TYR:CE2	1:D:296:ARG:HD2	2.54	0.42
1:A:69:ASN:ND2	1:A:96:GLU:O	2.44	0.42
1:B:195:ASP:OD2	1:F:140:ARG:NH2	2.52	0.42
1:A:175:ARG:HA	1:A:204:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ALA:HA	1:A:427:TRP:HA	2.02	0.42
1:A:492:VAL:HG12	1:D:492:VAL:HG11	2.01	0.42
1:F:5:LEU:HB3	1:F:6:ARG:H	1.71	0.42
1:A:129:HIS:CB	1:D:447:HIS:HB2	2.47	0.42
1:A:329:SER:HB2	1:A:354:CYS:HB3	2.02	0.42
1:B:88:LYS:HB2	1:E:188:GLU:O	2.19	0.42
1:D:220:ARG:HB2	1:D:220:ARG:NH1	2.35	0.42
1:F:225:GLN:HG2	1:F:229:GLU:OE1	2.19	0.42
1:C:337:HIS:O	1:C:343:GLU:HA	2.19	0.42
1:D:319:MET:HA	1:D:322:MET:HG2	2.02	0.42
1:E:475:ASN:HB2	1:E:476:GLU:OE1	2.20	0.42
1:D:181:ARG:NH2	1:D:185:ASN:OD1	2.53	0.41
1:D:349:HIS:NE2	2:D:586:HOH:O	2.37	0.41
1:F:5:LEU:HD11	1:F:321:VAL:HG13	2.02	0.41
1:C:494:TRP:HA	1:C:497:ARG:HG3	2.02	0.41
1:E:424:ARG:N	1:E:424:ARG:HD3	2.35	0.41
1:D:231:LEU:HD12	1:D:231:LEU:HA	1.87	0.41
1:E:154:ASP:HB3	1:E:157:VAL:HG23	2.00	0.41
1:F:337:HIS:O	1:F:343:GLU:HA	2.20	0.41
1:A:178:LYS:HB3	1:A:178:LYS:HE2	1.90	0.41
1:E:3:LEU:HD13	1:E:274:THR:HG22	2.01	0.41
1:D:241:VAL:HG13	1:D:365:GLU:HG2	2.02	0.41
1:A:95:LEU:HD23	1:A:95:LEU:HA	1.89	0.41
1:F:219:ILE:HG23	1:F:259:ARG:HG2	2.02	0.41
1:C:374:LYS:HD3	1:C:374:LYS:HA	1.83	0.41
1:D:247:GLU:OE2	1:D:255:ARG:NH2	2.41	0.41
1:E:244:GLY:O	1:E:251:ARG:NH1	2.54	0.41
1:A:181:ARG:NH2	1:A:185:ASN:OD1	2.53	0.41
1:C:47:PHE:CE2	1:C:169:VAL:HG21	2.56	0.41
1:C:355:PRO:HA	1:C:382:PHE:CZ	2.56	0.41
1:D:52:LYS:HD3	1:D:52:LYS:HA	1.93	0.41
1:E:51:PHE:CZ	1:E:53:SER:HA	2.56	0.41
1:E:225:GLN:O	1:E:229:GLU:HG3	2.21	0.41
1:E:99:LYS:HD3	1:E:99:LYS:HA	1.89	0.41
1:D:307:GLU:OE2	1:D:350:MET:HE2	2.21	0.40
1:B:71:SER:OG	1:B:73:GLN:HG2	2.21	0.40
1:B:196:LYS:HG3	2:B:505:HOH:O	2.21	0.40
1:E:137:ILE:HD12	1:E:137:ILE:HA	1.87	0.40
1:E:352:GLU:OE1	1:E:352:GLU:N	2.48	0.40
1:C:288:GLN:OE1	1:C:377:PRO:HA	2.21	0.40
1:A:339:GLU:HA	1:A:340:PRO:HD3	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:LEU:HD12	1:C:231:LEU:HA	1.88	0.40
1:C:412:LYS:HA	1:C:413:PRO:HD3	1.97	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	494/497 (99%)	480 (97%)	14 (3%)	0	100	100
1	B	493/497 (99%)	475 (96%)	18 (4%)	0	100	100
1	C	494/497 (99%)	473 (96%)	20 (4%)	1 (0%)	47	62
1	D	494/497 (99%)	479 (97%)	15 (3%)	0	100	100
1	E	492/497 (99%)	473 (96%)	19 (4%)	0	100	100
1	F	491/497 (99%)	474 (96%)	16 (3%)	1 (0%)	47	62
All	All	2958/2982 (99%)	2854 (96%)	102 (3%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	7	PRO
1	F	291	GLY

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	414/415 (100%)	405 (98%)	9 (2%)	52	71
1	B	413/415 (100%)	403 (98%)	10 (2%)	49	68
1	C	414/415 (100%)	401 (97%)	13 (3%)	40	60
1	D	414/415 (100%)	401 (97%)	13 (3%)	40	60
1	E	412/415 (99%)	401 (97%)	11 (3%)	44	65
1	F	411/415 (99%)	400 (97%)	11 (3%)	44	65
All	All	2478/2490 (100%)	2411 (97%)	67 (3%)	44	65

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	ASP
1	A	156	GLU
1	A	231	LEU
1	A	264	LEU
1	A	334	TYR
1	A	379	ARG
1	A	405	VAL
1	A	424	ARG
1	A	479	SER
1	B	26	LYS
1	B	268	LEU
1	B	320	LYS
1	B	324	ASP
1	B	334	TYR
1	B	363	ARG
1	B	379	ARG
1	B	405	VAL
1	B	424	ARG
1	B	457	THR
1	C	133	GLU
1	C	175	ARG
1	C	220	ARG
1	C	231	LEU
1	C	318	LEU
1	C	333	ASP
1	C	334	TYR
1	C	379	ARG
1	C	394	LEU
1	C	424	ARG
1	C	479	SER

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Mol	Chain	Res	Type
1	C	484	LYS
1	C	492	VAL
1	D	66	LEU
1	D	223	SER
1	D	240	ILE
1	D	246	GLN
1	D	268	LEU
1	D	318	LEU
1	D	334	TYR
1	D	335	THR
1	D	361	ARG
1	D	379	ARG
1	D	419	LYS
1	D	424	ARG
1	D	497	ARG
1	E	66	LEU
1	E	73	GLN
1	E	115	ASP
1	E	279	THR
1	E	334	TYR
1	E	363	ARG
1	E	379	ARG
1	E	405	VAL
1	E	424	ARG
1	E	479	SER
1	E	495	ARG
1	F	66	LEU
1	F	220	ARG
1	F	229	GLU
1	F	245	ARG
1	F	279	THR
1	F	334	TYR
1	F	370	SER
1	F	379	ARG
1	F	394	LEU
1	F	424	ARG
1	F	492	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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, 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	496/497 (99%)	-0.47	0 100 100	5, 12, 28, 43	0
1	B	495/497 (99%)	-0.41	6 (1%) 79 77	6, 14, 30, 44	0
1	C	496/497 (99%)	-0.44	4 (0%) 86 84	5, 12, 27, 63	0
1	D	496/497 (99%)	-0.37	8 (1%) 72 70	6, 15, 32, 48	0
1	E	494/497 (99%)	-0.04	24 (4%) 29 28	8, 18, 40, 63	0
1	F	493/497 (99%)	-0.13	20 (4%) 37 36	7, 17, 38, 57	0
All	All	2970/2982 (99%)	-0.31	62 (2%) 63 61	5, 14, 33, 63	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	248	GLY	5.3
1	E	241	VAL	5.2
1	E	247	GLU	5.1
1	F	22	GLU	4.9
1	C	4	SER	4.3
1	E	242	PRO	4.3
1	E	246	GLN	4.3
1	C	2	MET	4.2
1	E	243	ALA	4.1
1	F	246	GLN	3.9
1	E	245	ARG	3.9
1	F	414	GLU	3.8
1	E	250	VAL	3.8
1	D	221	ASP	3.7
1	E	223	SER	3.6
1	E	244	GLY	3.4
1	E	221	ASP	3.4
1	E	235	GLU	3.3
1	C	3	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	247	GLU	3.1
1	E	222	VAL	3.1
1	F	226	LYS	3.0
1	D	23	GLU	3.0
1	F	244	GLY	3.0
1	E	253	SER	2.9
1	F	250	VAL	2.8
1	F	249	PRO	2.8
1	E	255	ARG	2.8
1	E	249	PRO	2.7
1	B	43	SER	2.7
1	F	236	GLU	2.7
1	F	245	ARG	2.6
1	D	26	LYS	2.6
1	E	227	VAL	2.5
1	F	220	ARG	2.5
1	F	240	ILE	2.5
1	E	226	LYS	2.5
1	B	225	GLN	2.5
1	E	251	ARG	2.5
1	F	237	LEU	2.5
1	E	229	GLU	2.4
1	F	235	GLU	2.4
1	E	228	ASN	2.4
1	B	41	ARG	2.4
1	F	232	ASP	2.3
1	D	22	GLU	2.3
1	D	37	ASN	2.3
1	F	287	LYS	2.3
1	B	220	ARG	2.2
1	E	364	VAL	2.2
1	F	23	GLU	2.2
1	B	7	PRO	2.2
1	D	63	ARG	2.1
1	E	414	GLU	2.1
1	D	223	SER	2.1
1	F	224	GLU	2.1
1	C	324	ASP	2.1
1	B	115	ASP	2.1
1	F	233	GLU	2.0
1	F	26	LYS	2.0
1	E	360	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	41	ARG	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 monosaccharides 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.