Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:54 am BST

PDB ID	:	4R1P
Title	:	Crystal Structure of Thermophilic Geobacillus kaustophilus L-Arabinose isomerase with Mn2+
Authors	:	Choi, J.M.; Lee, Y.J.; Lee, D.W.; Lee, S.H.
Deposited on	:	2014-08-07
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 following versions of software and data (see references ⓘ) were used in the production of this report:

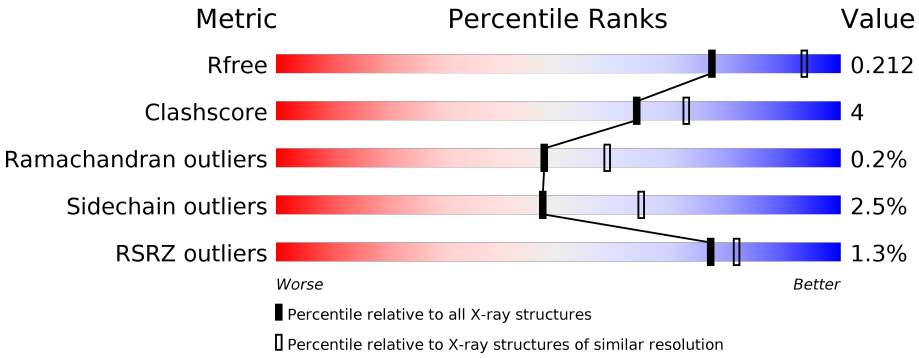
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	89% 10%
1	B	497	88% 10%
1	C	497	88% 10%
1	D	497	86% 12%
1	E	497	89% 10%
1	F	497	2% 87% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24768 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	494	Total	C	N	O	S	0	0	0
			3934	2503	688	722	21			
1	B	492	Total	C	N	O	S	0	0	0
			3919	2495	683	720	21			
1	C	495	Total	C	N	O	S	0	0	0
			3942	2508	689	723	22			
1	D	494	Total	C	N	O	S	0	0	0
			3934	2503	688	722	21			
1	E	495	Total	C	N	O	S	0	0	0
			3942	2508	689	723	22			
1	F	492	Total	C	N	O	S	0	0	0
			3920	2494	686	719	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 MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0

- Molecule 3 is water.

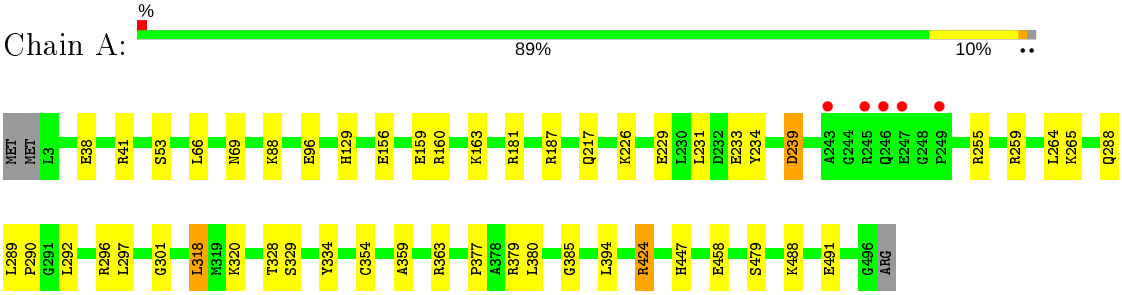
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	205	Total O 205 205	0	0
3	B	214	Total O 214 214	0	0
3	C	171	Total O 171 171	0	0
3	D	208	Total O 208 208	0	0
3	E	199	Total O 199 199	0	0
3	F	174	Total O 174 174	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

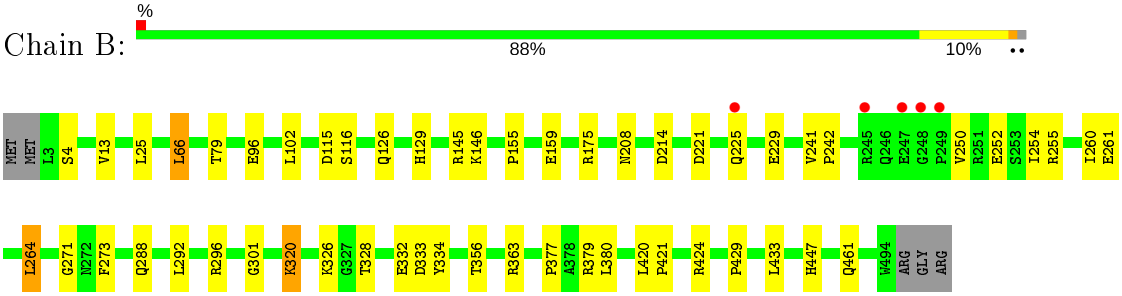
- Molecule 1: L-arabinose isomerase

Chain A:



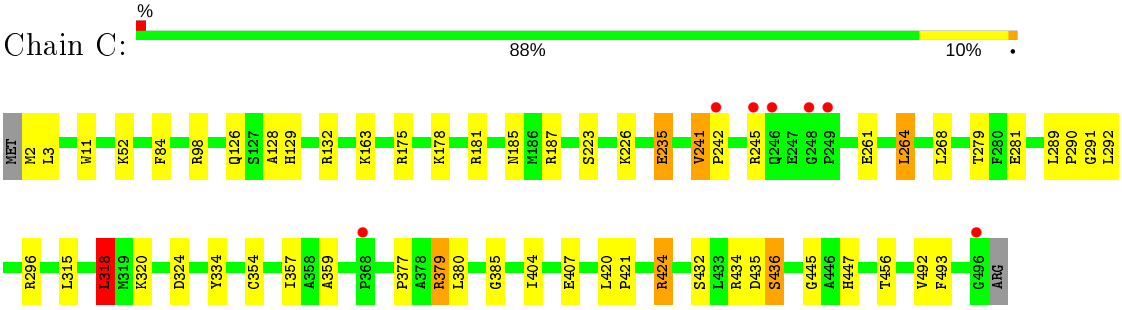
- Molecule 1: L-arabinose isomerase

Chain B:



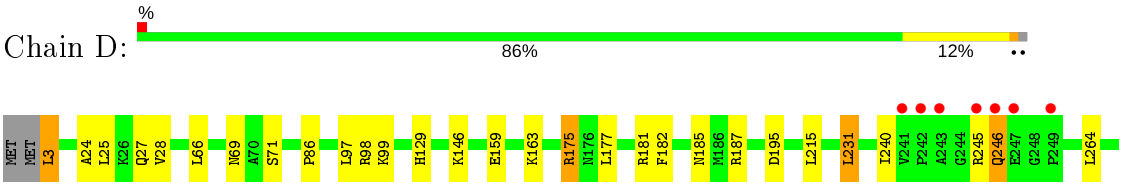
- Molecule 1: L-arabinose isomerase

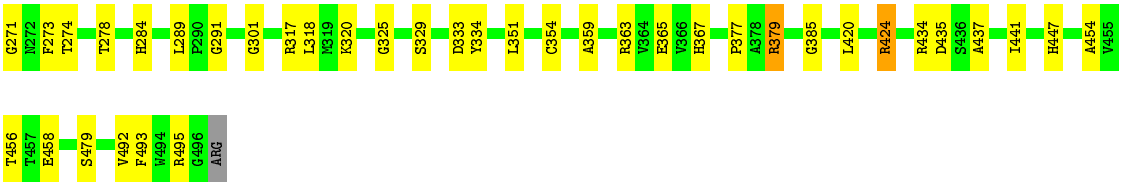
Chain C:



- Molecule 1: L-arabinose isomerase

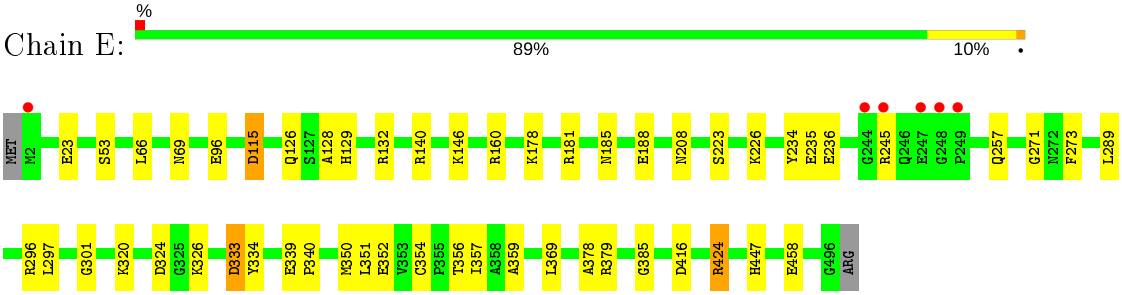
Chain D:





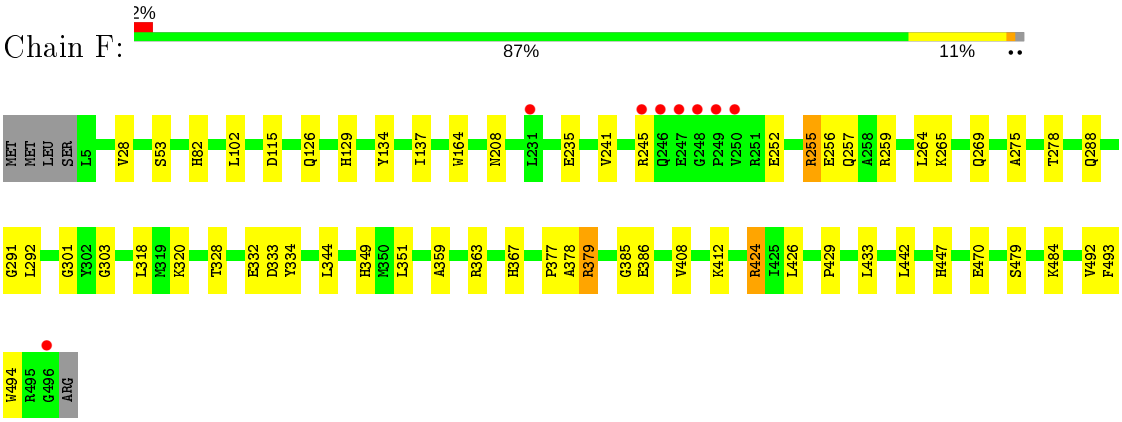
- Molecule 1: L-arabinose isomerase

Chain E:



- Molecule 1: L-arabinose isomerase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	223.66Å 153.12Å 91.24Å 90.00° 103.85° 90.00°	Depositor
Resolution (Å)	43.69 – 2.30 47.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (43.69-2.30) 98.9 (47.91-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.155 , 0.212 0.156 , 0.212	Depositor DCC
R_{free} test set	6588 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	24768	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.40	0/4033	0.54	0/5462
1	B	0.42	0/4018	0.56	1/5443 (0.0%)
1	C	0.40	0/4041	0.57	1/5472 (0.0%)
1	D	0.41	0/4033	0.55	0/5462
1	E	0.41	0/4041	0.54	0/5472
1	F	0.38	0/4019	0.55	0/5443
All	All	0.40	0/24185	0.55	2/32754 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	318	LEU	CA-CB-CG	7.35	132.22	115.30
1	B	320	LYS	CD-CE-NZ	5.20	123.66	111.70

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	3934	0	3824	32	0
1	B	3919	0	3808	31	0
1	C	3942	0	3833	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3934	0	3824	42	0
1	E	3942	0	3833	33	0
1	F	3920	0	3808	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	205	0	0	3	0
3	B	214	0	0	4	0
3	C	171	0	0	7	0
3	D	208	0	0	2	0
3	E	199	0	0	4	0
3	F	174	0	0	2	0
All	All	24768	0	22930	195	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 (195) 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:HIS:HB2	1:E:447:HIS:HB2	1.59	0.84
1:F:301:GLY:HA2	1:F:320:LYS:HD3	1.62	0.81
1:D:447:HIS:HB2	1:F:129:HIS:HB2	1.64	0.78
1:C:447:HIS:HB2	1:D:129:HIS:HB2	1.64	0.77
1:A:447:HIS:HB2	1:B:129:HIS:HB2	1.66	0.76
1:C:434:ARG:NH1	1:C:435:ASP:OD1	2.19	0.75
1:B:447:HIS:HB2	1:E:129:HIS:HB2	1.69	0.75
1:D:69:ASN:HD21	1:D:98:ARG:H	1.33	0.73
1:C:261:GLU:OE2	1:C:296:ARG:NH1	2.22	0.72
1:D:301:GLY:HA2	1:D:320:LYS:HE2	1.76	0.68
1:C:84:PHE:H	1:C:126:GLN:HE21	1.42	0.67
1:C:129:HIS:HB2	1:F:447:HIS:HB2	1.77	0.67
1:A:239:ASP:HB3	1:A:363:ARG:HG3	1.75	0.67
1:C:245:ARG:NH2	3:C:749:HOH:O	2.28	0.66
1:B:320:LYS:HE3	3:B:782:HOH:O	1.96	0.65
1:A:265:LYS:HG2	1:A:297:LEU:HD21	1.78	0.64
1:D:98:ARG:HH21	1:D:175:ARG:HH21	1.45	0.64
1:F:359:ALA:HB2	1:F:385:GLY:HA2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:PRO:O	1:D:379:ARG:NH2	2.31	0.63
1:E:359:ALA:HB2	1:E:385:GLY:HA2	1.81	0.63
1:C:320:LYS:HE3	3:C:756:HOH:O	1.99	0.62
1:E:301:GLY:HA2	1:E:320:LYS:HG2	1.81	0.62
1:A:38:GLU:OE1	1:A:41:ARG:NH2	2.26	0.62
1:D:98:ARG:HH21	1:D:175:ARG:NH2	1.98	0.61
1:A:359:ALA:HB2	1:A:385:GLY:HA2	1.82	0.61
1:C:126:GLN:HB2	1:C:129:HIS:CE1	2.36	0.61
1:B:261:GLU:OE2	1:B:296:ARG:NH1	2.33	0.60
1:D:379:ARG:NH1	3:D:717:HOH:O	2.23	0.60
1:D:289:LEU:HD23	1:D:351:LEU:HD12	1.84	0.60
1:A:181:ARG:HD3	3:F:609:HOH:O	2.01	0.60
1:B:320:LYS:HE2	1:B:328:THR:HB	1.84	0.60
1:D:278:THR:HG21	3:D:617:HOH:O	2.02	0.60
1:A:234:TYR:HE2	1:A:296:ARG:HD2	1.66	0.59
1:E:128:ALA:O	1:E:132:ARG:HD2	2.03	0.59
1:B:326:LYS:NZ	1:B:356:THR:O	2.27	0.58
1:F:126:GLN:HB2	1:F:129:HIS:CE1	2.38	0.58
1:B:155:PRO:O	1:B:159:GLU:HG2	2.03	0.58
1:A:289:LEU:HD12	1:A:290:PRO:HD2	1.86	0.57
1:C:424:ARG:N	1:C:424:ARG:HD3	2.19	0.57
1:A:160:ARG:NH1	1:A:458:GLU:OE1	2.37	0.57
1:A:226:LYS:NZ	1:A:229:GLU:OE2	2.38	0.57
1:D:3:LEU:HB3	1:D:317:ARG:HH12	1.69	0.57
1:E:333:ASP:OD2	1:E:333:ASP:N	2.38	0.57
1:B:301:GLY:HA2	1:B:320:LYS:HD2	1.87	0.56
1:D:181:ARG:NH2	1:D:185:ASN:OD1	2.35	0.56
1:A:66:LEU:HD13	1:A:96:GLU:HG2	1.87	0.56
1:F:344:LEU:HD13	1:F:426:LEU:HG	1.87	0.56
1:A:320:LYS:HE2	1:A:328:THR:HB	1.88	0.56
1:E:352:GLU:OE1	1:E:352:GLU:N	2.39	0.55
1:A:301:GLY:HA2	1:A:320:LYS:HD2	1.89	0.55
1:D:420:LEU:HD23	1:D:424:ARG:HD2	1.88	0.55
1:C:359:ALA:HB2	1:C:385:GLY:HA2	1.88	0.55
1:C:128:ALA:O	1:C:132:ARG:HD2	2.06	0.55
1:A:234:TYR:CE2	1:A:296:ARG:HD2	2.42	0.55
1:D:146:LYS:NZ	1:D:458:GLU:OE1	2.38	0.55
1:F:278:THR:HG21	3:F:730:HOH:O	2.08	0.54
1:C:181:ARG:HD3	3:E:757:HOH:O	2.08	0.54
1:C:492:VAL:HG23	1:F:492:VAL:HG21	1.90	0.54
1:B:332:GLU:OE2	1:B:447:HIS:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:288:GLN:OE1	1:F:377:PRO:HA	2.07	0.54
1:E:126:GLN:HB2	1:E:129:HIS:CE1	2.42	0.54
1:C:315:LEU:HA	1:C:318:LEU:HD22	1.90	0.53
1:A:88:LYS:HB2	1:E:188:GLU:O	2.08	0.53
1:A:320:LYS:HE3	3:A:790:HOH:O	2.07	0.53
1:A:424:ARG:HD3	1:A:424:ARG:N	2.23	0.53
1:C:289:LEU:HD12	1:C:290:PRO:HD2	1.91	0.53
1:D:175:ARG:HH11	1:D:175:ARG:HB3	1.73	0.53
1:A:129:HIS:HB2	1:E:447:HIS:CB	2.33	0.53
1:C:279:THR:HG21	3:C:748:HOH:O	2.09	0.53
1:C:178:LYS:NZ	3:C:706:HOH:O	2.42	0.52
1:D:359:ALA:HB2	1:D:385:GLY:HA2	1.91	0.52
1:D:329:SER:HB2	1:D:354:CYS:HB3	1.92	0.51
1:C:235:GLU:HG2	3:C:749:HOH:O	2.11	0.50
1:B:96:GLU:HG3	3:B:773:HOH:O	2.12	0.50
1:D:177:LEU:HG	1:D:274:THR:CG2	2.41	0.50
1:C:223:SER:HB3	1:C:226:LYS:HG3	1.94	0.49
1:C:420:LEU:HD12	1:C:421:PRO:HD2	1.93	0.49
1:A:233:GLU:OE2	1:A:296:ARG:NH2	2.37	0.49
1:E:181:ARG:NH2	1:E:185:ASN:OD1	2.45	0.49
1:F:134:TYR:O	1:F:137:ILE:HG22	2.13	0.49
1:F:470:GLU:HB2	1:F:494:TRP:CD1	2.47	0.49
1:F:320:LYS:NZ	1:F:328:THR:O	2.38	0.48
1:E:115:ASP:OD2	1:E:115:ASP:N	2.38	0.48
1:F:265:LYS:O	1:F:269:GLN:HG3	2.12	0.48
1:B:225:GLN:O	1:B:229:GLU:HG3	2.13	0.48
1:C:404:ILE:HD13	1:C:445:GLY:HA2	1.95	0.48
1:D:240:ILE:HB	1:D:245:ARG:HD3	1.96	0.48
1:A:292:LEU:HD13	1:A:380:LEU:HG	1.95	0.48
1:E:234:TYR:CE2	1:E:296:ARG:HD2	2.49	0.48
1:E:146:LYS:NZ	1:E:458:GLU:OE2	2.40	0.48
1:B:126:GLN:HB2	1:B:129:HIS:CE1	2.48	0.47
1:B:208:ASN:HB3	1:D:187:ARG:HG2	1.96	0.47
1:E:289:LEU:HD23	1:E:351:LEU:HD12	1.95	0.47
1:C:11:TRP:CE2	1:C:52:LYS:HE3	2.50	0.47
1:C:181:ARG:NH2	1:C:185:ASN:OD1	2.45	0.47
1:F:241:VAL:HG12	1:F:363:ARG:NH2	2.30	0.47
1:D:492:VAL:HG21	1:F:492:VAL:HG23	1.96	0.47
1:A:255:ARG:HD3	1:A:259:ARG:NH2	2.29	0.47
1:D:163:LYS:HE3	1:D:456:THR:HG21	1.97	0.47
1:F:256:GLU:OE2	1:F:259:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:PRO:HG2	1:B:433:LEU:HA	1.97	0.46
1:C:11:TRP:CD2	1:C:52:LYS:HE3	2.50	0.46
1:E:354:CYS:O	1:E:357:ILE:HG12	2.15	0.46
1:E:223:SER:OG	1:E:226:LYS:HG2	2.16	0.46
1:B:66:LEU:HD22	1:B:96:GLU:HG2	1.98	0.46
1:B:13:VAL:HG22	1:B:79:THR:HG22	1.98	0.46
1:C:377:PRO:O	1:C:379:ARG:NH2	2.48	0.46
1:F:332:GLU:OE2	1:F:447:HIS:HD2	1.99	0.45
1:A:156:GLU:O	1:A:159:GLU:HG2	2.16	0.45
1:C:264:LEU:O	1:C:268:LEU:HG	2.17	0.45
1:B:292:LEU:HD13	1:B:380:LEU:HG	1.99	0.45
1:E:235:GLU:OE2	1:E:245:ARG:NH1	2.50	0.45
1:A:329:SER:HB2	1:A:354:CYS:HB3	1.98	0.44
1:E:324:ASP:HB2	3:E:610:HOH:O	2.16	0.44
1:B:420:LEU:HD12	1:B:421:PRO:HD2	2.00	0.44
1:F:429:PRO:HG2	1:F:433:LEU:HA	2.00	0.44
1:C:493:PHE:HA	1:F:492:VAL:HG11	2.00	0.44
1:E:350:MET:HE2	1:E:369:LEU:HD21	1.99	0.44
1:F:408:VAL:HG12	1:F:429:PRO:HA	1.99	0.44
1:F:367:HIS:O	1:F:377:PRO:HD2	2.18	0.44
1:D:325:GLY:H	1:D:454:ALA:HB1	1.83	0.44
1:F:252:GLU:OE1	1:F:255:ARG:HD2	2.18	0.44
1:A:163:LYS:HE3	3:A:675:HOH:O	2.17	0.44
1:D:274:THR:OG1	1:D:317:ARG:NE	2.51	0.43
1:C:407:GLU:OE2	3:C:732:HOH:O	2.21	0.43
1:E:53:SER:HB2	3:E:772:HOH:O	2.18	0.43
1:C:163:LYS:HE3	1:C:456:THR:HG21	2.00	0.43
1:D:69:ASN:HD21	1:D:97:LEU:HA	1.82	0.43
1:E:257:GLN:HG3	1:E:378:ALA:HB3	1.99	0.43
1:D:71:SER:O	1:D:99:LYS:NZ	2.51	0.43
1:F:386:GLU:HB3	1:F:412:LYS:HG2	2.01	0.43
1:C:492:VAL:HG21	1:D:492:VAL:HG23	2.01	0.43
1:E:326:LYS:NZ	1:E:356:THR:O	2.33	0.43
1:B:145:ARG:HD2	3:B:614:HOH:O	2.19	0.43
1:B:250:VAL:O	1:B:254:ILE:HG13	2.18	0.43
1:C:163:LYS:NZ	1:C:324:ASP:OD1	2.51	0.43
1:E:69:ASN:ND2	1:E:96:GLU:O	2.47	0.43
1:D:333:ASP:O	1:F:129:HIS:HB3	2.19	0.43
1:F:424:ARG:HD3	1:F:424:ARG:N	2.34	0.42
1:D:492:VAL:HG11	1:F:493:PHE:HA	2.01	0.42
1:C:292:LEU:HD13	1:C:380:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:434:ARG:NH1	1:D:435:ASP:OD1	2.52	0.42
1:F:442:LEU:HD13	1:F:484:LYS:HE2	2.01	0.42
1:C:447:HIS:CB	1:D:129:HIS:HB2	2.43	0.42
1:D:24:ALA:O	1:D:28:VAL:HG13	2.20	0.42
1:F:332:GLU:OE1	1:F:349:HIS:CD2	2.72	0.42
1:B:115:ASP:N	1:B:115:ASP:OD1	2.53	0.42
1:A:187:ARG:HG2	1:F:208:ASN:HB3	2.01	0.42
1:C:432:SER:O	1:C:436:SER:HB3	2.18	0.42
1:D:271:GLY:HA3	1:D:273:PHE:CE2	2.54	0.42
1:B:241:VAL:HG23	1:B:363:ARG:NH1	2.33	0.42
1:F:292:LEU:HB2	1:F:379:ARG:HA	2.02	0.42
1:A:318:LEU:HD12	1:A:318:LEU:HA	1.86	0.42
1:D:231:LEU:HD12	1:D:231:LEU:HA	1.85	0.42
1:B:252:GLU:OE1	1:B:255:ARG:HD2	2.20	0.42
1:B:271:GLY:HA3	1:B:273:PHE:CE2	2.54	0.42
1:E:297:LEU:HA	1:E:297:LEU:HD23	1.71	0.42
1:A:41:ARG:NE	3:A:638:HOH:O	2.48	0.41
1:A:488:LYS:O	1:A:491:GLU:HB3	2.21	0.41
1:D:182:PHE:CE2	1:D:215:LEU:HB2	2.55	0.41
1:D:25:LEU:HD23	1:D:25:LEU:HA	1.81	0.41
1:B:214:ASP:OD1	1:D:284:HIS:NE2	2.41	0.41
1:E:271:GLY:HA3	1:E:273:PHE:CE2	2.55	0.41
1:C:98:ARG:O	1:C:175:ARG:NH1	2.43	0.41
1:E:424:ARG:HD3	1:E:424:ARG:N	2.35	0.41
1:F:102:LEU:HD12	1:F:164:TRP:CD2	2.56	0.41
1:D:363:ARG:HD3	1:D:365:GLU:OE2	2.20	0.41
1:A:69:ASN:ND2	1:A:96:GLU:O	2.44	0.41
1:B:102:LEU:HD12	1:B:146:LYS:HG2	2.02	0.41
1:B:241:VAL:HA	1:B:242:PRO:HD3	1.91	0.41
1:E:447:HIS:CD2	1:E:447:HIS:H	2.38	0.41
1:C:261:GLU:OE1	1:C:296:ARG:HD3	2.21	0.41
1:B:25:LEU:HD23	1:B:25:LEU:HA	1.93	0.41
1:B:288:GLN:OE1	1:B:377:PRO:HA	2.20	0.41
1:A:359:ALA:HB2	1:A:385:GLY:CA	2.49	0.41
1:C:187:ARG:HG2	1:E:208:ASN:HB3	2.03	0.41
1:D:367:HIS:O	1:D:377:PRO:HD2	2.21	0.41
1:D:437:ALA:O	1:D:441:ILE:HG13	2.20	0.41
1:F:257:GLN:HG3	1:F:378:ALA:HB3	2.03	0.41
1:F:28:VAL:HB	1:F:82:HIS:CD2	2.56	0.41
1:A:288:GLN:OE1	1:A:377:PRO:HA	2.22	0.40
1:B:461:GLN:HG2	3:B:744:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:VAL:HA	1:C:242:PRO:HD2	1.79	0.40
1:C:2:MET:HB3	1:C:3:LEU:H	1.55	0.40
1:C:492:VAL:HG11	1:D:493:PHE:HA	2.03	0.40
1:D:195:ASP:OD2	1:E:140:ARG:NH2	2.51	0.40
1:E:339:GLU:HA	1:E:340:PRO:HD3	1.96	0.40
1:C:279:THR:HG22	1:C:281:GLU:H	1.86	0.40
1:F:291:GLY:HA3	1:F:351:LEU:HD13	2.03	0.40
1:B:260:ILE:O	1:B:264:LEU:HB2	2.21	0.40
1:C:354:CYS:O	1:C:357:ILE:HG12	2.21	0.40
1:E:178:LYS:HB3	1:E:178:LYS:HE2	1.84	0.40
1:F:275:ALA:HA	1:F:303:GLY:O	2.21	0.40
1:E:23:GLU:HG2	3:E:770:HOH:O	2.20	0.40
1:C:324:ASP:HB2	3:C:635:HOH:O	2.20	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	492/497 (99%)	480 (98%)	12 (2%)	0	100	100
1	B	490/497 (99%)	475 (97%)	15 (3%)	0	100	100
1	C	493/497 (99%)	478 (97%)	14 (3%)	1 (0%)	47	58
1	D	492/497 (99%)	477 (97%)	11 (2%)	4 (1%)	19	23
1	E	493/497 (99%)	478 (97%)	15 (3%)	0	100	100
1	F	490/497 (99%)	479 (98%)	10 (2%)	1 (0%)	47	58
All	All	2950/2982 (99%)	2867 (97%)	77 (3%)	6 (0%)	47	58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	495	ARG
1	D	246	GLN
1	F	53	SER
1	C	291	GLY
1	D	291	GLY
1	D	86	PRO

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	412/415 (99%)	401 (97%)	11 (3%)	44	61
1	B	411/415 (99%)	401 (98%)	10 (2%)	49	66
1	C	413/415 (100%)	405 (98%)	8 (2%)	57	73
1	D	412/415 (99%)	399 (97%)	13 (3%)	39	54
1	E	413/415 (100%)	404 (98%)	9 (2%)	52	69
1	F	410/415 (99%)	399 (97%)	11 (3%)	44	61
All	All	2471/2490 (99%)	2409 (98%)	62 (2%)	47	65

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	217	GLN
1	A	231	LEU
1	A	239	ASP
1	A	264	LEU
1	A	318	LEU
1	A	334	TYR
1	A	379	ARG
1	A	394	LEU
1	A	424	ARG
1	A	479	SER
1	B	4	SER
1	B	66	LEU

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Mol	Chain	Res	Type
1	B	116	SER
1	B	175	ARG
1	B	221	ASP
1	B	264	LEU
1	B	333	ASP
1	B	334	TYR
1	B	379	ARG
1	B	424	ARG
1	C	235	GLU
1	C	241	VAL
1	C	264	LEU
1	C	318	LEU
1	C	334	TYR
1	C	379	ARG
1	C	424	ARG
1	C	436	SER
1	D	3	LEU
1	D	27	GLN
1	D	66	LEU
1	D	159	GLU
1	D	175	ARG
1	D	231	LEU
1	D	246	GLN
1	D	264	LEU
1	D	318	LEU
1	D	334	TYR
1	D	379	ARG
1	D	424	ARG
1	D	479	SER
1	E	66	LEU
1	E	115	ASP
1	E	160	ARG
1	E	236	GLU
1	E	333	ASP
1	E	334	TYR
1	E	379	ARG
1	E	416	ASP
1	E	424	ARG
1	F	115	ASP
1	F	235	GLU
1	F	245	ARG
1	F	255	ARG

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Mol	Chain	Res	Type
1	F	264	LEU
1	F	318	LEU
1	F	333	ASP
1	F	334	TYR
1	F	379	ARG
1	F	424	ARG
1	F	479	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	126	GLN
1	D	69	ASN
1	F	73	GLN
1	F	272	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	494/497 (99%)	-0.39	5 (1%)	82 86	2, 9, 26, 48	0
1	B	492/497 (98%)	-0.35	5 (1%)	82 86	2, 9, 25, 40	0
1	C	495/497 (99%)	-0.32	7 (1%)	75 80	3, 12, 32, 44	0
1	D	494/497 (99%)	-0.33	7 (1%)	75 80	2, 10, 31, 51	0
1	E	495/497 (99%)	-0.27	6 (1%)	79 83	3, 11, 32, 47	0
1	F	492/497 (98%)	-0.29	8 (1%)	72 77	4, 12, 31, 51	0
All	All	2962/2982 (99%)	-0.32	38 (1%)	77 81	2, 11, 30, 51	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	GLN	3.9
1	D	241	VAL	3.7
1	A	245	ARG	3.7
1	F	245	ARG	3.5
1	F	246	GLN	3.5
1	E	249	PRO	3.4
1	C	245	ARG	3.3
1	D	245	ARG	3.3
1	D	246	GLN	3.1
1	F	248	GLY	3.1
1	A	249	PRO	3.1
1	D	249	PRO	3.0
1	E	248	GLY	2.9
1	E	247	GLU	2.9
1	B	249	PRO	2.8
1	B	248	GLY	2.6
1	B	245	ARG	2.6
1	E	245	ARG	2.6
1	D	242	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	246	GLN	2.5
1	F	231	LEU	2.5
1	B	225	GLN	2.5
1	F	247	GLU	2.4
1	C	248	GLY	2.4
1	D	247	GLU	2.3
1	C	496	GLY	2.3
1	F	496	GLY	2.3
1	C	249	PRO	2.2
1	F	249	PRO	2.1
1	B	247	GLU	2.1
1	F	250	VAL	2.1
1	C	368	PRO	2.1
1	A	247	GLU	2.1
1	D	243	ALA	2.1
1	C	242	PRO	2.1
1	E	244	GLY	2.1
1	E	2	MET	2.0
1	A	243	ALA	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 carbohydrates 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	E	501	1/1	0.99	0.13	13,13,13,13	0
2	MN	F	501	1/1	0.99	0.10	13,13,13,13	0
2	MN	A	501	1/1	0.99	0.10	12,12,12,12	0
2	MN	C	501	1/1	1.00	0.10	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	B	501	1/1	1.00	0.11	12,12,12,12	0
2	MN	D	501	1/1	1.00	0.11	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.