



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:11 PM GMT

PDB ID : 4QK0
Title : Crystal structure of Ara127N-Se, a GH127 beta-L-arabinofuranosidase from Geobacillus Stearothermophilus T6
Authors : Lansky, S.; Salama, R.; Dann, R.; Shner, I.; Manjasetty, B.; Belrhali, H.; Shoham, Y.; Shoham, G.
Deposited on : 2014-06-05
Resolution : 2.26 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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

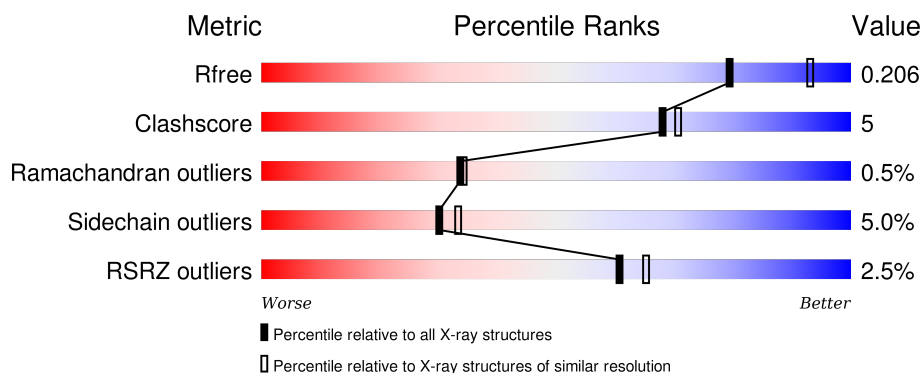
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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. 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	648	<div> <div>2%</div> <div>86%</div> <div>9%</div> <div>• •</div> </div>
1	B	648	<div> <div>4%</div> <div>85%</div> <div>11%</div> <div>• •</div> </div>
1	C	648	<div> <div>2%</div> <div>85%</div> <div>11%</div> <div>• •</div> </div>
1	D	648	<div> <div>2%</div> <div>87%</div> <div>10%</div> <div>• •</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22177 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 GH127 beta-L-arabinofuranoside.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	635	Total	C	N	O	S	Se	0	1	0
			5152	3297	880	949	11	15			
1	B	635	Total	C	N	O	S	Se	0	6	0
			5179	3316	883	952	11	17			
1	C	635	Total	C	N	O	S	Se	0	3	0
			5165	3306	883	949	11	16			
1	D	635	Total	C	N	O	S	Se	0	3	0
			5163	3304	881	952	11	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	EXPRESSION TAG	UNP B3EYN9
A	-2	HIS	-	EXPRESSION TAG	UNP B3EYN9
A	-1	HIS	-	EXPRESSION TAG	UNP B3EYN9
A	0	HIS	-	EXPRESSION TAG	UNP B3EYN9
A	1	HIS	-	EXPRESSION TAG	UNP B3EYN9
A	2	HIS	-	EXPRESSION TAG	UNP B3EYN9
B	-3	HIS	-	EXPRESSION TAG	UNP B3EYN9
B	-2	HIS	-	EXPRESSION TAG	UNP B3EYN9
B	-1	HIS	-	EXPRESSION TAG	UNP B3EYN9
B	0	HIS	-	EXPRESSION TAG	UNP B3EYN9
B	1	HIS	-	EXPRESSION TAG	UNP B3EYN9
B	2	HIS	-	EXPRESSION TAG	UNP B3EYN9
C	-3	HIS	-	EXPRESSION TAG	UNP B3EYN9
C	-2	HIS	-	EXPRESSION TAG	UNP B3EYN9
C	-1	HIS	-	EXPRESSION TAG	UNP B3EYN9
C	0	HIS	-	EXPRESSION TAG	UNP B3EYN9
C	1	HIS	-	EXPRESSION TAG	UNP B3EYN9
C	2	HIS	-	EXPRESSION TAG	UNP B3EYN9
D	-3	HIS	-	EXPRESSION TAG	UNP B3EYN9
D	-2	HIS	-	EXPRESSION TAG	UNP B3EYN9
D	-1	HIS	-	EXPRESSION TAG	UNP B3EYN9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	EXPRESSION TAG	UNP B3EYN9
D	1	HIS	-	EXPRESSION TAG	UNP B3EYN9
D	2	HIS	-	EXPRESSION TAG	UNP B3EYN9

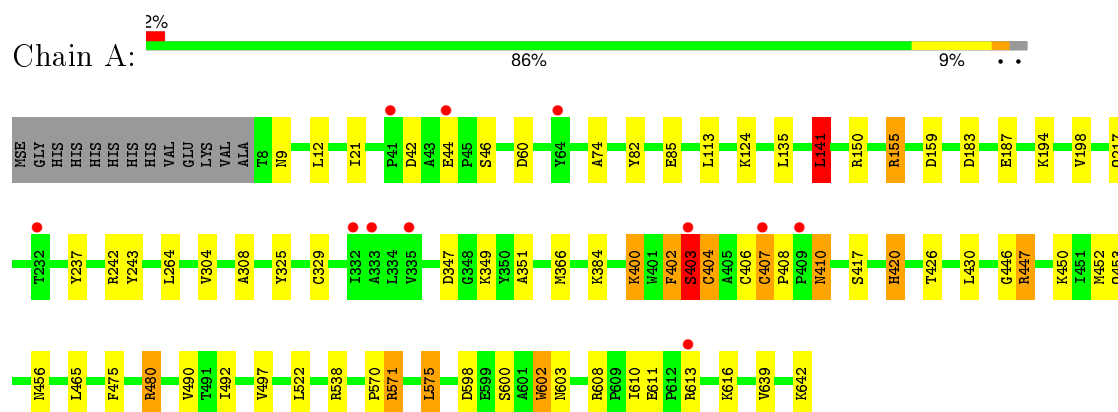
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	343	Total 343	O 343	0	0
2	B	311	Total 311	O 311	0	0
2	C	401	Total 401	O 401	0	0
2	D	463	Total 463	O 463	0	0

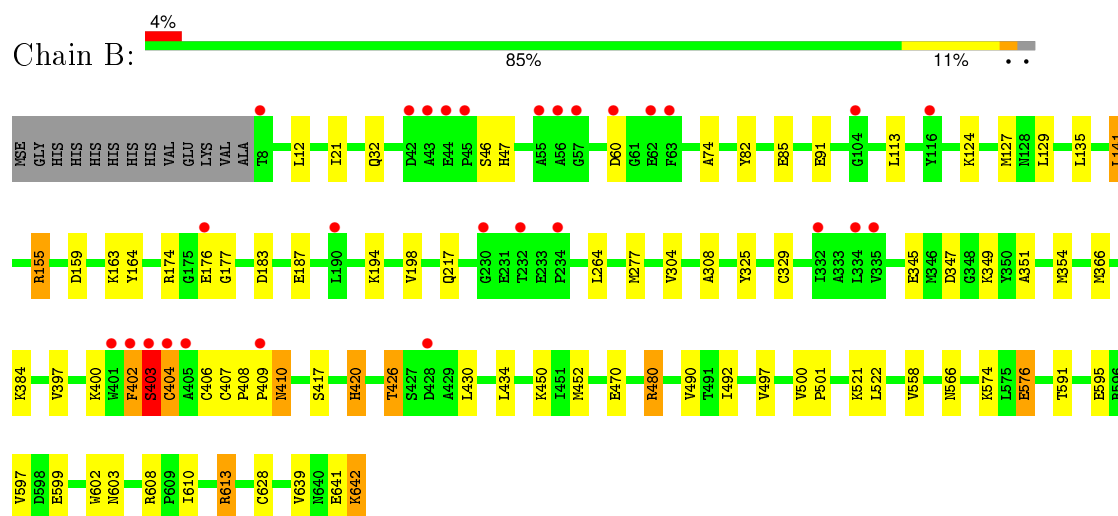
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

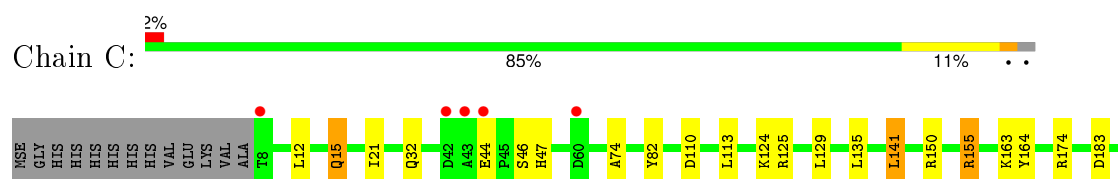
- Molecule 1: GH127 beta-L-arabinofuranoside



- Molecule 1: GH127 beta-L-arabinofuranoside

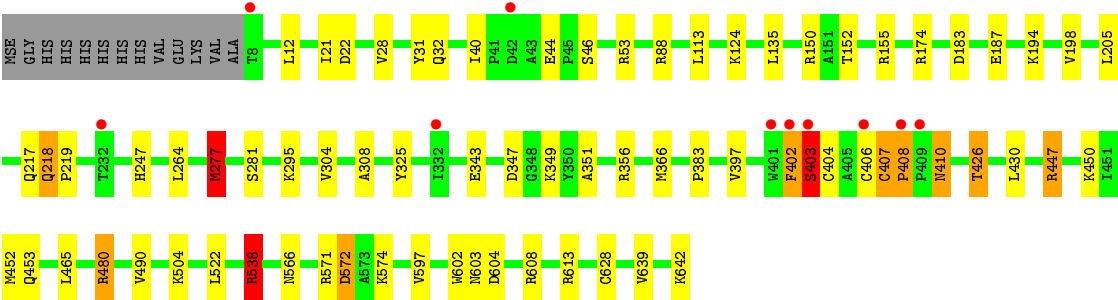
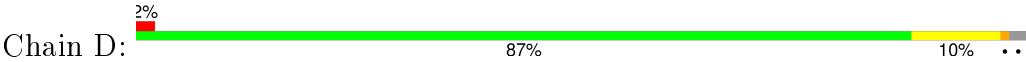


- Molecule 1: GH127 beta-L-arabinofuranoside





● Molecule 1: GH127 beta-L-arabinofuranoside



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.38Å 132.27Å 109.05Å 90.00° 113.06° 90.00°	Depositor
Resolution (Å)	40.00 – 2.26 39.97 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-2.26) 99.6 (39.97-2.26)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.157 , 0.200 0.170 , 0.206	Depositor DCC
R_{free} test set	6452 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.2	EDS
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 128249 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22177	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.18% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.80	0/5278	0.84	5/7137 (0.1%)
1	B	0.78	0/5320	0.82	3/7192 (0.0%)
1	C	0.85	0/5297	0.85	8/7161 (0.1%)
1	D	0.85	0/5295	0.87	9/7160 (0.1%)
All	All	0.82	0/21190	0.85	25/28650 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	538	ARG	NE-CZ-NH1	9.43	125.01	120.30
1	D	538	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	C	480	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	D	150	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	D	480	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	C	352	ASP	CB-CG-OD1	6.12	123.80	118.30
1	C	155	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	C	277	MSE	CG-SE-CE	5.79	111.65	98.90
1	D	480	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	538	ARG	CB-CG-CD	5.64	126.26	111.60
1	C	354[A]	MSE	CG-SE-CE	-5.56	86.67	98.90
1	C	354[B]	MSE	CG-SE-CE	-5.56	86.67	98.90
1	C	480	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	480	ARG	NE-CZ-NH2	-5.51	117.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	480	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	447	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	D	277	MSE	CG-SE-CE	5.31	110.59	98.90
1	C	548	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	D	53	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	572[A]	ASP	CA-C-O	-5.20	109.19	120.10
1	D	572[B]	ASP	CA-C-O	-5.20	109.19	120.10
1	B	608	ARG	CA-CB-CG	5.17	124.79	113.40
1	A	141	LEU	CA-CB-CG	5.15	127.15	115.30
1	A	575	LEU	CA-CB-CG	5.03	126.87	115.30
1	B	277	MSE	CB-CA-C	-5.02	100.36	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	572[A]	ASP	Mainchain
1	D	572[B]	ASP	Mainchain

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	5152	0	4996	40	0
1	B	5179	0	5036	46	0
1	C	5165	0	5018	59	0
1	D	5163	0	5008	54	0
2	A	343	0	0	14	0
2	B	311	0	0	17	0
2	C	401	0	0	18	0
2	D	463	0	0	11	0
All	All	22177	0	20058	190	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 5.

All (190) 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:642:LYS:HE2	1:D:642:LYS:HB3	1.44	0.98
1:A:329:CYS:SG	2:A:1019:HOH:O	2.22	0.97
1:C:642:LYS:HE2	1:D:642:LYS:CB	1.97	0.95
1:B:426:THR:HG21	2:B:895:HOH:O	1.65	0.94
1:B:595:GLU:OE1	1:B:642:LYS:HE3	1.75	0.87
1:D:571:ARG:CZ	1:D:642:LYS:HD3	2.04	0.86
1:A:456:ASN:HB3	2:A:784:HOH:O	1.76	0.85
1:D:277:MSE:HE2	1:D:277:MSE:HA	1.63	0.81
1:A:74:ALA:HB2	1:A:141:LEU:HD13	1.63	0.80
1:C:642:LYS:CE	1:D:642:LYS:HB3	2.11	0.79
1:C:641:GLU:OE1	2:C:1096:HOH:O	2.03	0.77
1:B:74:ALA:HB2	1:B:141:LEU:HD13	1.67	0.77
1:D:217:GLN:HG3	2:D:1127:HOH:O	1.83	0.77
1:C:281:SER:HB3	2:C:892:HOH:O	1.84	0.76
1:C:74:ALA:HB2	1:C:141:LEU:HD13	1.67	0.76
1:B:345:GLU:HG3	2:B:757:HOH:O	1.84	0.76
1:B:174:ARG:HB3	2:B:984:HOH:O	1.87	0.74
1:B:127[B]:MSE:HA	1:B:127[B]:MSE:HE3	1.69	0.74
1:C:47:HIS:ND1	2:C:1081:HOH:O	2.23	0.72
1:C:603:ASN:HB3	2:C:1046:HOH:O	1.89	0.72
1:D:343:GLU:OE1	2:D:1131:HOH:O	2.08	0.72
1:D:571:ARG:HB2	1:D:642:LYS:HD2	1.71	0.72
1:D:356:ARG:NH2	2:D:913:HOH:O	2.23	0.71
1:A:404:CYS:SG	2:A:1018:HOH:O	2.48	0.71
1:B:602:TRP:O	1:B:603:ASN:OD1	2.09	0.71
1:D:571:ARG:NH2	1:D:642:LYS:HD3	2.06	0.70
1:D:277:MSE:CE	1:D:277:MSE:HA	2.21	0.70
1:D:602:TRP:O	1:D:603:ASN:OD1	2.10	0.70
1:A:384:LYS:HE3	2:B:871:HOH:O	1.92	0.69
1:A:452:MSE:HE3	2:A:937:HOH:O	1.92	0.69
1:C:452[A]:MSE:HE3	2:C:926:HOH:O	1.91	0.68
1:D:22:ASP:OD1	2:D:1003:HOH:O	2.12	0.68
1:C:247:HIS:H	1:C:247:HIS:CD2	2.13	0.67
1:A:603:ASN:HB2	2:A:809:HOH:O	1.94	0.67
1:A:406:CYS:O	1:A:410:ASN:HB2	1.93	0.67
1:D:406:CYS:O	1:D:410:ASN:HB2	1.94	0.66
1:B:406:CYS:O	1:B:410:ASN:HB2	1.95	0.66
1:C:566:ASN:HD21	1:C:597:VAL:HB	1.62	0.64
1:D:247:HIS:H	1:D:247:HIS:CD2	2.13	0.64
1:B:641:GLU:OE1	2:B:981:HOH:O	2.15	0.64
1:B:177:GLY:HA3	2:B:920:HOH:O	1.98	0.62
1:D:566:ASN:HD21	1:D:597:VAL:HB	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:602:TRP:HA	1:C:608:ARG:NH1	2.15	0.62
1:C:464:ARG:HD3	2:C:1033:HOH:O	1.98	0.62
1:D:356:ARG:CZ	2:D:913:HOH:O	2.48	0.61
1:C:15:GLN:NE2	2:C:944:HOH:O	2.33	0.61
1:A:602:TRP:HA	1:A:608:ARG:NH1	2.15	0.61
1:A:150:ARG:NH1	2:A:1015:HOH:O	2.34	0.60
1:A:616:LYS:HE2	2:A:1017:HOH:O	2.02	0.59
2:C:847:HOH:O	1:D:538:ARG:HD3	2.01	0.59
1:C:277:MSE:HE3	1:C:277:MSE:HA	1.85	0.59
1:B:566:ASN:HD21	1:B:597:VAL:HB	1.68	0.57
1:B:91:GLU:HG2	2:B:925:HOH:O	2.04	0.57
1:C:452[A]:MSE:CE	2:C:926:HOH:O	2.51	0.57
1:C:642:LYS:HA	2:C:891:HOH:O	2.06	0.56
1:C:110:ASP:OD2	1:C:125:ARG:NH2	2.38	0.56
1:A:351:ALA:HB3	1:A:480:ARG:HD3	1.87	0.56
1:C:603:ASN:HB3	2:C:979:HOH:O	2.06	0.56
1:B:351:ALA:HB3	1:B:480:ARG:HD3	1.89	0.55
1:A:217:GLN:HG3	2:A:840:HOH:O	2.05	0.55
1:D:571:ARG:NE	1:D:642:LYS:CD	2.70	0.55
1:D:351:ALA:HB3	1:D:480:ARG:HD3	1.89	0.55
1:B:558:VAL:HG23	1:C:174:ARG:HD3	1.89	0.54
1:C:406:CYS:O	1:C:410:ASN:HB2	2.08	0.54
1:D:504:LYS:HG3	2:D:1058:HOH:O	2.08	0.53
1:B:127[B]:MSE:CE	1:B:127[B]:MSE:HA	2.37	0.53
1:C:155:ARG:NE	2:C:999:HOH:O	2.39	0.53
1:B:566:ASN:HD21	1:B:597:VAL:H	1.57	0.53
1:C:129:LEU:HD13	2:C:1085:HOH:O	2.09	0.53
1:B:347:ASP:OD2	1:B:349:LYS:HE2	2.09	0.52
1:B:613:ARG:NH1	1:B:613:ARG:HB2	2.24	0.52
1:C:351:ALA:HB3	1:C:480:ARG:HD3	1.91	0.52
1:C:32:GLN:NE2	1:C:409:PRO:HB3	2.25	0.52
1:D:571:ARG:CZ	1:D:642:LYS:CD	2.83	0.52
1:A:603:ASN:CB	2:A:809:HOH:O	2.54	0.52
1:B:32:GLN:NE2	1:B:409:PRO:HB3	2.25	0.52
1:D:218:GLN:HG3	1:D:219:PRO:HA	1.91	0.52
1:A:347:ASP:OD2	1:A:349:LYS:HE2	2.10	0.51
1:D:566:ASN:HD21	1:D:597:VAL:H	1.59	0.51
1:D:347:ASP:OD2	1:D:349:LYS:HE2	2.10	0.51
1:C:382:TRP:CE3	1:D:538:ARG:HD2	2.46	0.51
1:B:85:GLU:OE1	1:B:420:HIS:HE1	1.94	0.51
1:B:576:GLU:OE1	1:B:591:THR:OG1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:HB2	1:A:183:ASP:HB2	1.93	0.50
1:A:570:PRO:HB3	1:A:571:ARG:NH2	2.28	0.49
1:D:571:ARG:NE	1:D:642:LYS:HD2	2.28	0.49
1:C:44:GLU:OE1	1:C:402:PHE:HB2	2.13	0.48
1:D:295:LYS:HE3	2:D:789:HOH:O	2.13	0.48
1:D:135:LEU:HB2	1:D:183:ASP:HB2	1.95	0.48
1:C:641:GLU:O	1:C:642:LYS:HB2	2.14	0.48
1:C:491:THR:HG22	1:C:496:LYS:HD2	1.95	0.48
1:C:12:LEU:HD12	1:C:21:ILE:HD12	1.95	0.48
1:D:383:PRO:O	2:D:987:HOH:O	2.20	0.48
1:C:296[B]:ARG:HD2	1:C:317:PHE:CZ	2.48	0.48
1:D:490:VAL:HG22	1:D:522:LEU:HD23	1.96	0.48
1:C:226:LYS:HG3	1:C:231:GLU:HB2	1.96	0.47
1:A:456:ASN:CB	2:A:784:HOH:O	2.50	0.47
1:C:296[B]:ARG:HH22	1:D:604:ASP:HA	1.78	0.47
1:B:521:LYS:HD3	2:B:820:HOH:O	2.14	0.47
1:C:308:ALA:HA	1:C:325:TYR:CD1	2.50	0.47
1:B:135:LEU:HB2	1:B:183:ASP:HB2	1.96	0.47
1:C:642:LYS:CE	1:D:642:LYS:CB	2.79	0.47
1:A:85:GLU:OE1	1:A:420:HIS:HE1	1.97	0.47
1:C:492:ILE:HD12	1:C:497:VAL:HG21	1.96	0.47
1:D:447:ARG:NH1	2:D:1159:HOH:O	2.48	0.47
1:B:384:LYS:HG2	2:B:955:HOH:O	2.14	0.47
1:C:602:TRP:HA	1:C:608:ARG:HH12	1.79	0.46
1:C:296[B]:ARG:CD	1:C:317:PHE:CZ	2.99	0.46
1:A:264:LEU:HD11	1:A:304:VAL:HG21	1.97	0.46
1:D:402:PHE:O	1:D:403:SER:CB	2.64	0.46
1:A:400:LYS:O	2:A:959:HOH:O	2.21	0.46
1:C:640:ASN:ND2	2:C:970:HOH:O	2.41	0.46
1:A:598:ASP:OD1	1:A:600:SER:HB2	2.14	0.46
1:C:150:ARG:NH1	2:C:1086:HOH:O	2.46	0.46
1:D:88:ARG:HH12	1:D:152:THR:HG22	1.79	0.46
1:D:566:ASN:HD21	1:D:597:VAL:CB	2.28	0.46
1:A:242:ARG:HD2	2:A:985:HOH:O	2.16	0.46
1:D:406:CYS:O	1:D:407:CYS:C	2.54	0.46
1:D:264:LEU:HD11	1:D:304:VAL:HG21	1.98	0.46
1:A:12:LEU:HD12	1:A:21:ILE:HD12	1.96	0.46
1:B:264:LEU:HD11	1:B:304:VAL:HG21	1.98	0.46
1:B:492:ILE:HD12	1:B:497:VAL:HG21	1.98	0.45
1:B:12:LEU:HD12	1:B:21:ILE:HD12	1.98	0.45
1:C:642:LYS:HE2	1:D:642:LYS:HB2	1.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ALA:HA	1:B:325:TYR:CD1	2.51	0.45
1:D:490:VAL:HG22	1:D:522:LEU:CD2	2.46	0.45
1:C:566:ASN:HD21	1:C:597:VAL:CB	2.29	0.45
1:C:135:LEU:HB2	1:C:183:ASP:HB2	1.99	0.45
1:A:490:VAL:HG22	1:A:522:LEU:HD23	1.98	0.45
1:A:402:PHE:O	1:A:403:SER:CB	2.65	0.45
1:C:598:ASP:OD1	1:C:600:SER:HB2	2.16	0.45
1:A:602:TRP:HA	1:A:608:ARG:HH12	1.80	0.45
1:C:642:LYS:HE2	1:D:642:LYS:CD	2.47	0.44
1:A:490:VAL:HG22	1:A:522:LEU:CD2	2.48	0.44
1:C:402:PHE:O	1:C:403:SER:CB	2.65	0.44
1:A:453:GLN:HG2	1:A:465:LEU:CD2	2.48	0.44
1:C:183:ASP:OD2	2:C:1085:HOH:O	2.21	0.44
1:C:490:VAL:HG22	1:C:522:LEU:HD23	2.00	0.44
1:C:486:ARG:NH2	1:C:529:GLU:OE2	2.48	0.44
1:C:566:ASN:HD21	1:C:597:VAL:H	1.66	0.44
1:D:28:VAL:HG12	1:D:32[B]:GLN:NE2	2.32	0.44
1:B:155:ARG:NH1	1:B:159:ASP:OD1	2.50	0.44
1:A:447:ARG:HH22	1:A:475:PHE:HD2	1.60	0.43
1:C:264:LEU:HD11	1:C:304:VAL:HG21	2.00	0.43
1:C:406:CYS:O	1:C:407:CYS:C	2.57	0.43
1:D:452:MSE:HB2	1:D:452:MSE:HE3	1.94	0.43
1:B:402:PHE:O	1:B:403:SER:CB	2.67	0.43
1:D:426:THR:HG21	2:D:1059:HOH:O	2.17	0.43
1:D:31:TYR:CZ	1:D:40:ILE:HD13	2.54	0.43
1:D:32[B]:GLN:NE2	1:D:408:PRO:HB2	2.34	0.43
1:A:406:CYS:O	1:A:407:CYS:C	2.58	0.43
1:B:85:GLU:OE1	1:B:420:HIS:CE1	2.71	0.43
1:B:397:VAL:HA	1:B:628:CYS:SG	2.59	0.42
1:B:217:GLN:O	2:B:785:HOH:O	2.21	0.42
1:A:308:ALA:HA	1:A:325:TYR:CD1	2.54	0.42
1:C:453:GLN:HG2	1:C:465:LEU:CD2	2.49	0.42
1:A:446:GLY:N	2:A:1016:HOH:O	2.38	0.42
1:D:566:ASN:ND2	1:D:597:VAL:HB	2.32	0.42
1:B:490:VAL:HG22	1:B:522:LEU:CD2	2.49	0.42
1:B:595:GLU:OE1	1:B:642:LYS:CE	2.59	0.42
1:B:47:HIS:CD2	2:B:863:HOH:O	2.72	0.42
1:D:12:LEU:HD12	1:D:21:ILE:HD12	2.02	0.42
1:C:82:TYR:CD2	1:C:417:SER:HB3	2.55	0.42
1:B:129:LEU:HA	2:B:953:HOH:O	2.19	0.42
1:D:308:ALA:HA	1:D:325:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:MSE:HE3	2:B:731:HOH:O	2.19	0.41
1:A:42:ASP:N	1:A:42:ASP:OD1	2.40	0.41
1:C:291:GLU:OE2	1:C:349:LYS:HE3	2.20	0.41
1:B:354[A]:MSE:HE3	1:B:434:LEU:HD21	2.01	0.41
1:A:492:ILE:HD12	1:A:497:VAL:HG21	2.00	0.41
1:C:238:ASP:HB3	2:C:984:HOH:O	2.20	0.41
1:D:281:SER:O	2:D:1027:HOH:O	2.22	0.41
1:B:404:CYS:SG	2:B:988:HOH:O	2.62	0.41
1:B:329:CYS:SG	2:B:989:HOH:O	2.62	0.41
1:A:82:TYR:CD2	1:A:417:SER:HB3	2.55	0.41
1:B:82:TYR:CD2	1:B:417:SER:HB3	2.56	0.41
1:B:500:VAL:N	1:B:501:PRO:HD2	2.36	0.41
1:C:32:GLN:HE22	1:C:409:PRO:HB3	1.86	0.41
1:B:490:VAL:HG22	1:B:522:LEU:HD23	2.03	0.41
1:C:641:GLU:O	1:C:642:LYS:CB	2.69	0.41
1:C:163:LYS:NZ	2:C:1024:HOH:O	2.52	0.41
1:D:397:VAL:HA	1:D:628:CYS:SG	2.61	0.41
1:B:176:GLU:HA	2:B:977:HOH:O	2.21	0.40
1:A:9:ASN:HA	2:A:1021:HOH:O	2.21	0.40
1:D:205:LEU:HD21	1:D:277:MSE:CE	2.51	0.40
1:B:452:MSE:CE	2:B:731:HOH:O	2.69	0.40
1:A:155:ARG:NH1	1:A:159:ASP:OD1	2.53	0.40
1:D:453:GLN:HG2	1:D:465:LEU:CD2	2.52	0.40
1:A:453:GLN:HG2	1:A:465:LEU:HD23	2.04	0.40
1:A:237:TYR:CD2	1:A:243:TYR:HB2	2.57	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	634/648 (98%)	612 (96%)	19 (3%)	3 (0%)	34 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	639/648 (99%)	618 (97%)	18 (3%)	3 (0%)	34	34
1	C	636/648 (98%)	614 (96%)	19 (3%)	3 (0%)	34	34
1	D	636/648 (98%)	614 (96%)	19 (3%)	3 (0%)	34	34
All	All	2545/2592 (98%)	2458 (97%)	75 (3%)	12 (0%)	34	34

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	GLU
1	B	187	GLU
1	C	187	GLU
1	D	187	GLU
1	A	403	SER
1	C	403	SER
1	D	403	SER
1	B	403	SER
1	A	408	PRO
1	B	408	PRO
1	C	408	PRO
1	D	408	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	535/530 (101%)	507 (95%)	28 (5%)	29	31
1	B	540/530 (102%)	510 (94%)	30 (6%)	26	27
1	C	537/530 (101%)	513 (96%)	24 (4%)	34	38
1	D	537/530 (101%)	512 (95%)	25 (5%)	32	36
All	All	2149/2120 (101%)	2042 (95%)	107 (5%)	30	33

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	46	SER
1	A	60	ASP
1	A	113	LEU
1	A	124	LYS
1	A	141	LEU
1	A	155	ARG
1	A	194	LYS
1	A	198	VAL
1	A	366	MSE
1	A	400	LYS
1	A	402	PHE
1	A	403	SER
1	A	404	CYS
1	A	407	CYS
1	A	410	ASN
1	A	420	HIS
1	A	426	THR
1	A	430	LEU
1	A	450	LYS
1	A	571	ARG
1	A	575	LEU
1	A	602	TRP
1	A	610	ILE
1	A	611	GLU
1	A	613	ARG
1	A	639	VAL
1	A	642	LYS
1	B	46	SER
1	B	60	ASP
1	B	113	LEU
1	B	124	LYS
1	B	141	LEU
1	B	155	ARG
1	B	163	LYS
1	B	164	TYR
1	B	194	LYS
1	B	198	VAL
1	B	366[A]	MSE
1	B	366[B]	MSE
1	B	400	LYS
1	B	402	PHE
1	B	403	SER

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Mol	Chain	Res	Type
1	B	404	CYS
1	B	407	CYS
1	B	410	ASN
1	B	420	HIS
1	B	426	THR
1	B	430	LEU
1	B	450	LYS
1	B	470	GLU
1	B	574	LYS
1	B	576	GLU
1	B	599	GLU
1	B	610	ILE
1	B	613	ARG
1	B	639	VAL
1	B	642	LYS
1	C	15	GLN
1	C	46	SER
1	C	113	LEU
1	C	124	LYS
1	C	141	LEU
1	C	164	TYR
1	C	194	LYS
1	C	198	VAL
1	C	366	MSE
1	C	400	LYS
1	C	402	PHE
1	C	403	SER
1	C	404	CYS
1	C	407	CYS
1	C	410	ASN
1	C	430	LEU
1	C	447	ARG
1	C	450	LYS
1	C	496	LYS
1	C	574	LYS
1	C	602	TRP
1	C	610	ILE
1	C	611	GLU
1	C	616	LYS
1	D	44	GLU
1	D	46	SER
1	D	113	LEU

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Mol	Chain	Res	Type
1	D	124	LYS
1	D	155	ARG
1	D	174	ARG
1	D	194	LYS
1	D	198	VAL
1	D	218	GLN
1	D	277	MSE
1	D	366	MSE
1	D	402	PHE
1	D	403	SER
1	D	404	CYS
1	D	407	CYS
1	D	410	ASN
1	D	426	THR
1	D	430	LEU
1	D	447	ARG
1	D	450	LYS
1	D	538	ARG
1	D	574	LYS
1	D	608	ARG
1	D	613	ARG
1	D	639	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	HIS
1	A	377	ASN
1	A	410	ASN
1	A	420	HIS
1	A	456	ASN
1	A	515	GLN
1	B	377	ASN
1	B	410	ASN
1	B	420	HIS
1	B	515	GLN
1	B	566	ASN
1	C	15	GLN
1	C	217	GLN
1	C	247	HIS
1	C	377	ASN
1	C	456	ASN

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Mol	Chain	Res	Type
1	C	515	GLN
1	C	566	ASN
1	D	217	GLN
1	D	247	HIS
1	D	377	ASN
1	D	410	ASN
1	D	456	ASN
1	D	515	GLN
1	D	566	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	621/648 (95%)	-0.34	11 (1%) 71 75	18, 32, 63, 108	0
1	B	621/648 (95%)	-0.03	28 (4%) 37 41	19, 37, 84, 118	0
1	C	621/648 (95%)	-0.38	13 (2%) 67 71	14, 27, 64, 101	0
1	D	621/648 (95%)	-0.47	10 (1%) 74 77	15, 25, 56, 99	0
All	All	2484/2592 (95%)	-0.30	62 (2%) 61 65	14, 30, 70, 118	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	409	PRO	7.0
1	A	409	PRO	5.8
1	B	404	CYS	5.8
1	B	403	SER	5.6
1	B	62	GLU	5.3
1	B	42	ASP	4.7
1	B	60	ASP	4.5
1	B	43	ALA	4.1
1	C	403	SER	4.0
1	D	409	PRO	3.9
1	B	401	TRP	3.7
1	C	405	ALA	3.6
1	C	409	PRO	3.6
1	C	8	THR	3.5
1	D	8	THR	3.4
1	D	406	CYS	3.4
1	B	63	PHE	3.4
1	B	44	GLU	3.4
1	B	104	GLY	3.3
1	B	232	THR	3.3
1	A	403	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	335	VAL	3.1
1	C	42	ASP	3.0
1	A	407	CYS	3.0
1	B	176	GLU	3.0
1	A	44	GLU	3.0
1	D	403	SER	2.9
1	B	230	GLY	2.8
1	C	402	PHE	2.7
1	C	407	CYS	2.7
1	B	405	ALA	2.7
1	C	234	PRO	2.7
1	A	332	ILE	2.6
1	B	116	TYR	2.6
1	C	44	GLU	2.6
1	B	57	GLY	2.5
1	D	401	TRP	2.5
1	B	428	ASP	2.4
1	A	41	PRO	2.4
1	B	402	PHE	2.3
1	B	55	ALA	2.3
1	B	335	VAL	2.3
1	B	234	PRO	2.3
1	D	402	PHE	2.3
1	C	447	ARG	2.3
1	A	232	THR	2.3
1	B	8	THR	2.2
1	D	408	PRO	2.2
1	B	45	PRO	2.2
1	D	42	ASP	2.2
1	A	333	ALA	2.1
1	B	332	ILE	2.1
1	B	190	LEU	2.1
1	B	56	ALA	2.1
1	C	43	ALA	2.1
1	C	233	GLU	2.1
1	A	64	TYR	2.1
1	C	60	ASP	2.1
1	A	613	ARG	2.0
1	B	334	LEU	2.0
1	D	332	ILE	2.0
1	D	232	THR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.