Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 02:55 PM JST

PDB ID	:	7CT6
Title	:	Crystal structure of GCL from Deinococcus metallilatus
Authors	:	Kim, J.H.; Kim, J.S.
Deposited on	:	2020-08-18
Resolution	:	2.10 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
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)	:	2.36
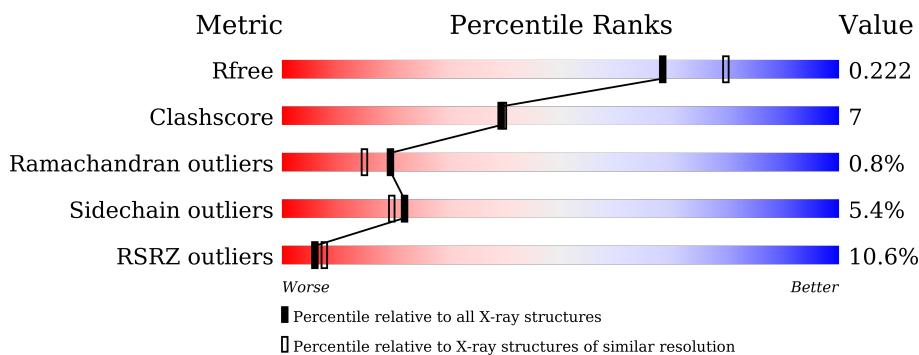
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
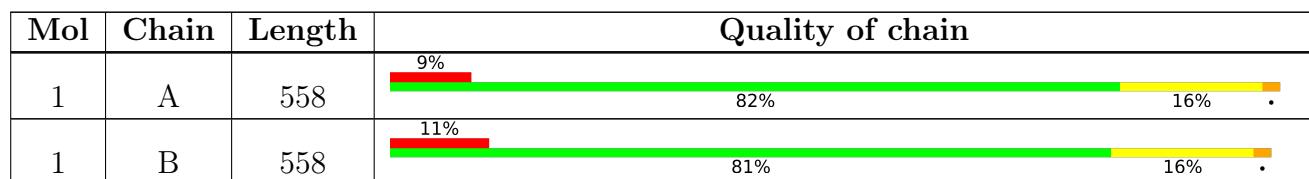
The reported resolution of this entry is 2.10 Å.

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	Percentile Ranks	Value
Rfree		0.222
Clashscore		7
Ramachandran outliers		0.8%
Sidechain outliers		5.4%
RSRZ outliers		10.6%

Worse   Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	558	9% 82% 16% •
1	B	558	11% 81% 16% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8916 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 Glyoxylate carboligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	Se	0	0	0
			4295	2743	748	781	4	19			
1	B	558	Total	C	N	O	S	Se	0	0	0
			4295	2743	748	781	4	19			
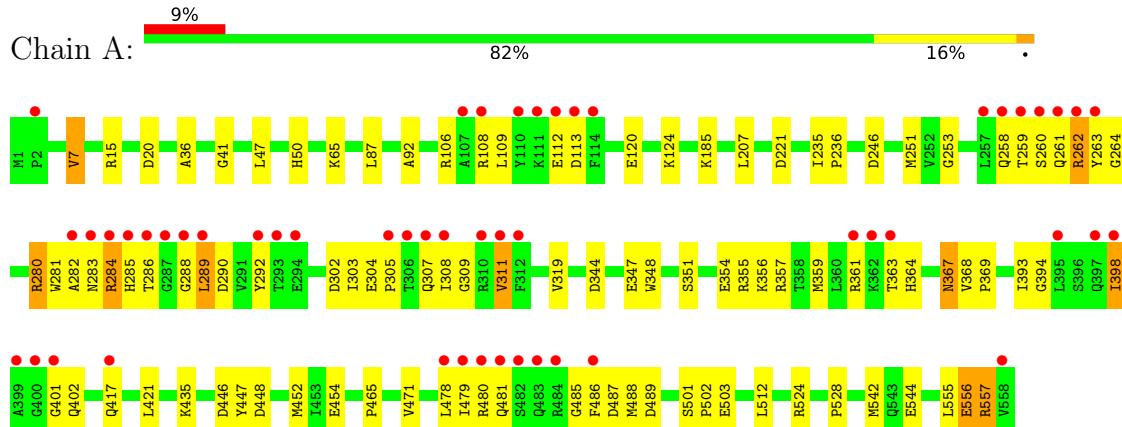
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	163	Total	O	0	0
			163	163		
2	B	163	Total	O	0	0
			163	163		
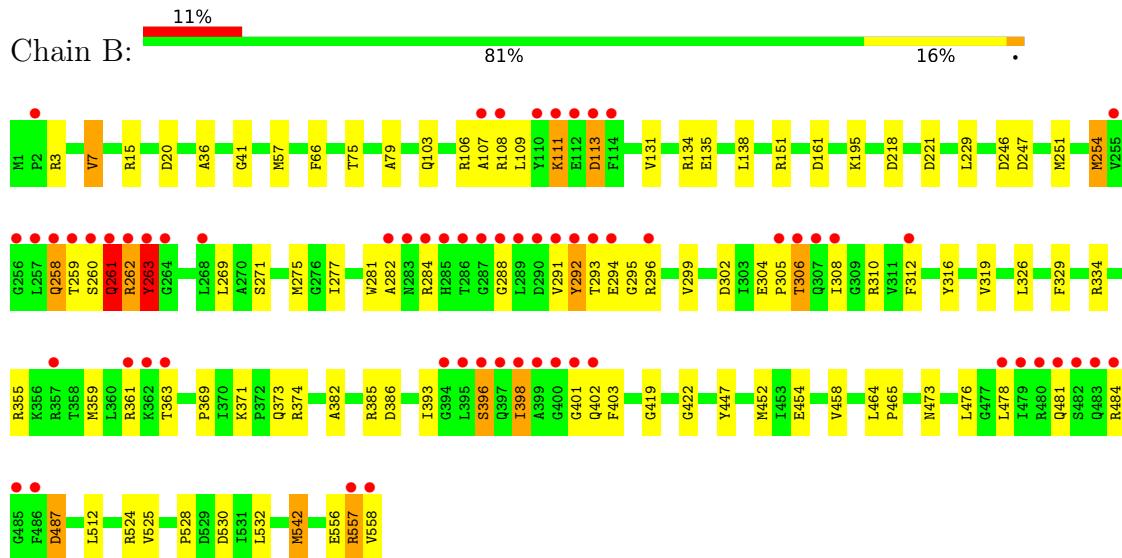
3 Residue-property plots ⓘ

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: Glyoxylate carboligase

Chain A:

• Molecule 1: Glyoxylate carboligase

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.06Å 106.47Å 89.09Å 90.00° 124.09° 90.00°	Depositor
Resolution (Å)	46.50 – 2.10 46.51 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.50-2.10) 98.4 (46.51-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.176 , 0.215 0.186 , 0.222	Depositor DCC
R_{free} test set	2631 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.0	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.8	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8916	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.38	0/4375	0.57	0/5916
1	B	0.38	0/4375	0.55	0/5916
All	All	0.38	0/8750	0.56	0/11832

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	263	TYR	Peptide

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	4295	0	4308	62	1
1	B	4295	0	4308	65	0
2	A	163	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	163	0	0	7	0
All	All	8916	0	8616	127	1

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 (127) 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:280:ARG:HA	1:A:308:ILE:HD11	1.57	0.84
1:A:544:GLU:OE1	2:A:601:HOH:O	1.94	0.83
1:B:151:ARG:NH1	2:B:601:HOH:O	2.09	0.81
1:B:229:LEU:HD21	1:B:334:ARG:HG3	1.64	0.79
1:B:263:TYR:HD1	1:B:263:TYR:H	1.34	0.76
1:A:92:ALA:HB1	1:A:417:GLN:HG2	1.69	0.75
1:A:302:ASP:OD1	2:A:602:HOH:O	2.06	0.73
1:B:361:ARG:HB3	1:B:401:GLY:HA2	1.73	0.70
1:A:487:ASP:O	2:A:603:HOH:O	2.09	0.70
1:B:284:ARG:HH22	1:B:292:TYR:HB3	1.55	0.70
1:B:271:SER:O	1:B:296:ARG:NH1	2.26	0.68
1:A:344:ASP:OD2	2:A:604:HOH:O	2.10	0.68
1:A:354:GLU:OE1	1:A:357:ARG:NH1	2.26	0.68
1:A:284:ARG:HH22	1:A:289:LEU:HD13	1.58	0.67
1:A:454:GLU:OE1	2:A:605:HOH:O	2.14	0.66
1:B:258:GLN:HB2	1:B:282:ALA:HB3	1.77	0.66
1:B:308:ILE:N	2:B:607:HOH:O	2.28	0.65
1:A:259:THR:HB	1:A:289:LEU:HD22	1.78	0.65
1:B:221:ASP:OD1	2:B:602:HOH:O	2.15	0.64
1:A:465:PRO:HB2	1:A:542:MSE:HG3	1.79	0.64
1:B:293:THR:HG22	1:B:295:GLY:H	1.64	0.61
1:B:305:PRO:HA	2:B:607:HOH:O	2.01	0.60
1:A:421:LEU:HD22	1:A:448:ASP:HB2	1.83	0.60
1:A:398:ILE:H	1:A:398:ILE:HD13	1.68	0.58
1:B:284:ARG:CZ	1:B:288:GLY:HA2	2.33	0.58
1:A:185:LYS:HD2	1:A:303:ILE:HD11	1.85	0.58
1:B:57:MSE:HE1	1:B:458:VAL:HG21	1.85	0.58
1:A:305:PRO:HG2	1:A:319:VAL:HG22	1.85	0.57
1:A:355:ARG:O	1:A:359:MSE:HG2	2.04	0.57
1:B:281:TRP:H	1:B:308:ILE:HD11	1.70	0.57
1:B:487:ASP:O	2:B:603:HOH:O	2.18	0.57
1:B:302:ASP:O	1:B:305:PRO:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:MSE:HE3	1:B:299:VAL:HG11	1.87	0.56
1:B:259:THR:OG1	1:B:284:ARG:HA	2.06	0.55
1:A:485:GLY:HA2	1:A:488:MSE:HE2	1.88	0.55
1:B:396:SER:HB2	1:B:403:PHE:CZ	2.41	0.55
1:B:20:ASP:OD2	2:B:604:HOH:O	2.18	0.55
1:B:310:ARG:HA	1:B:310:ARG:HH11	1.72	0.54
1:A:361:ARG:HD2	1:A:402:GLN:H	1.73	0.54
1:A:258:GLN:HG2	1:A:282:ALA:HB3	1.89	0.54
1:A:356:LYS:NZ	2:A:611:HOH:O	2.38	0.54
1:B:106:ARG:HA	1:B:109:LEU:HG	1.90	0.54
1:B:304:GLU:C	1:B:306:THR:H	2.12	0.53
1:B:259:THR:HG21	1:B:284:ARG:HE	1.73	0.53
1:B:465:PRO:HB2	1:B:542:MSE:HG2	1.91	0.53
1:A:367:ASN:OD1	1:A:367:ASN:N	2.41	0.53
1:A:15:ARG:NH1	1:A:41:GLY:O	2.41	0.52
1:A:106:ARG:HA	1:A:109:LEU:HB2	1.90	0.52
1:A:261:GLN:O	1:A:289:LEU:HD21	2.10	0.52
1:A:65:LYS:HE3	1:A:435:LYS:HG2	1.92	0.52
1:A:246:ASP:O	1:A:251:MSE:HE3	2.10	0.52
1:A:280:ARG:HH12	1:A:417:GLN:CD	2.13	0.52
1:A:292:TYR:HB3	1:A:311:VAL:HG23	1.92	0.51
1:A:284:ARG:NH2	1:A:289:LEU:HD13	2.26	0.51
1:A:305:PRO:HA	1:A:308:ILE:HG22	1.94	0.50
1:B:310:ARG:HA	1:B:310:ARG:NH1	2.25	0.50
1:B:195:LYS:HD3	1:B:316:TYR:CE1	2.46	0.50
1:B:246:ASP:O	1:B:251:MSE:HE2	2.12	0.50
1:B:294:GLU:H	1:B:294:GLU:CD	2.14	0.50
1:A:50:HIS:HB3	1:A:452:MSE:HE1	1.93	0.50
1:A:260:SER:HB3	1:A:264:GLY:HA2	1.94	0.50
1:A:7:VAL:HG13	1:A:36:ALA:HB2	1.93	0.49
1:A:280:ARG:NH1	1:A:417:GLN:OE1	2.45	0.49
1:A:478:LEU:HA	2:A:653:HOH:O	2.11	0.49
1:A:502:PRO:HG2	1:A:503:GLU:OE1	2.13	0.49
1:A:285:HIS:O	1:A:285:HIS:ND1	2.43	0.48
1:A:471:VAL:HB	1:A:555:LEU:HD11	1.95	0.48
1:B:374:ARG:HG2	1:B:528:PRO:HB3	1.96	0.48
1:B:195:LYS:HD3	1:B:316:TYR:CZ	2.49	0.48
1:A:236:PRO:HD2	1:A:253:GLY:O	2.14	0.48
1:B:108:ARG:NE	1:B:113:ASP:OD2	2.47	0.48
1:A:363:THR:O	1:A:402:GLN:NE2	2.27	0.47
1:A:284:ARG:HD2	1:A:285:HIS:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ILE:HG22	2:A:607:HOH:O	2.14	0.47
1:B:363:THR:HB	1:B:373:GLN:HB3	1.96	0.47
1:B:454:GLU:OE1	2:B:605:HOH:O	2.21	0.47
1:B:557:ARG:HA	1:B:557:ARG:HD2	1.61	0.47
1:A:92:ALA:HB1	1:A:417:GLN:CG	2.41	0.46
1:B:305:PRO:HD2	1:B:319:VAL:HG22	1.97	0.46
1:B:512:LEU:HD21	1:B:524:ARG:HB2	1.97	0.46
1:A:512:LEU:HD22	1:A:524:ARG:CZ	2.45	0.46
1:B:512:LEU:HD22	1:B:524:ARG:CZ	2.45	0.46
1:B:247:ASP:OD2	1:B:385:ARG:NH1	2.42	0.46
1:B:260:SER:C	1:B:261:GLN:HG3	2.37	0.45
1:A:304:GLU:N	1:A:305:PRO:HD3	2.32	0.44
1:B:422:GLY:O	1:B:452:MSE:HG3	2.17	0.44
1:B:135:GLU:HG2	1:B:138:LEU:HG	1.99	0.44
1:B:277:ILE:HD13	1:B:326:LEU:HD21	1.99	0.44
1:B:251:MSE:O	1:B:251:MSE:HE3	2.18	0.44
1:B:305:PRO:HD2	1:B:319:VAL:HG13	1.99	0.44
1:A:368:VAL:HG22	1:A:528:PRO:HD3	2.00	0.43
1:A:20:ASP:OD2	2:A:606:HOH:O	2.21	0.43
1:B:106:ARG:HD3	1:B:134:ARG:O	2.18	0.43
1:B:103:GLN:HB2	1:B:161:ASP:OD1	2.19	0.43
1:A:108:ARG:CZ	1:A:113:ASP:HB2	2.49	0.43
1:A:465:PRO:HB2	1:A:542:MSE:CG	2.47	0.43
1:B:261:GLN:HB2	1:B:262:ARG:H	1.65	0.43
1:A:361:ARG:NE	1:A:401:GLY:HA2	2.33	0.43
1:A:288:GLY:HA2	1:A:292:TYR:OH	2.19	0.43
1:B:382:ALA:HB2	1:B:532:LEU:HD12	2.00	0.42
1:B:66:PHE:CD1	1:B:218:ASP:HB2	2.54	0.42
1:B:7:VAL:HG13	1:B:36:ALA:HB2	2.02	0.42
1:A:304:GLU:O	1:A:308:ILE:HG22	2.19	0.42
1:B:107:ALA:O	1:B:111:LYS:HE2	2.19	0.42
1:A:120:GLU:O	1:A:124:LYS:HG3	2.19	0.42
1:B:310:ARG:C	1:B:312:PHE:H	2.23	0.42
1:B:254:MSE:HE2	1:B:254:MSE:HB3	1.78	0.41
1:B:355:ARG:O	1:B:359:MSE:HG2	2.20	0.41
1:A:284:ARG:HD3	1:A:285:HIS:CD2	2.54	0.41
1:A:465:PRO:CB	1:A:542:MSE:HG3	2.48	0.41
1:A:369:PRO:HB2	1:A:556:GLU:HB3	2.01	0.41
1:B:275:MSE:HE1	1:B:329:PHE:CZ	2.56	0.41
1:B:258:GLN:NE2	1:B:291:VAL:HG21	2.36	0.41
1:A:364:HIS:HA	2:A:654:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ARG:HD2	1:B:41:GLY:O	2.21	0.41
1:A:185:LYS:CD	1:A:303:ILE:HD11	2.51	0.41
1:B:369:PRO:HB3	1:B:476:LEU:HD11	2.01	0.41
1:B:371:LYS:HD3	1:B:556:GLU:OE2	2.20	0.41
1:A:207:LEU:HD13	1:A:235:ILE:HD12	2.03	0.40
1:A:262:ARG:HA	1:A:290:ASP:OD2	2.20	0.40
1:B:75:THR:O	1:B:79:ALA:HB3	2.21	0.40
1:A:283:ASN:HB3	1:A:286:THR:HA	2.03	0.40
1:B:473:ASN:O	1:B:558:VAL:HB	2.22	0.40
1:B:398:ILE:H	1:B:398:ILE:HG12	1.63	0.40
1:A:446:ASP:OD1	1:A:446:ASP:N	2.52	0.40
1:B:304:GLU:C	1:B:306:THR:N	2.74	0.40
1:B:525:VAL:HG13	1:B:530:ASP:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ARG:NH2	1:A:348:TRP:O[2_556]	2.01	0.19

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	556/558 (100%)	533 (96%)	18 (3%)	5 (1%)	17	12
1	B	556/558 (100%)	533 (96%)	19 (3%)	4 (1%)	22	18
All	All	1112/1116 (100%)	1066 (96%)	37 (3%)	9 (1%)	19	15

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	557	ARG
1	A	263	TYR
1	A	557	ARG
1	B	484	ARG
1	A	309	GLY
1	B	261	GLN
1	A	311	VAL
1	B	419	GLY
1	A	394	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	448/429 (104%)	424 (95%)	24 (5%)	22	20
1	B	448/429 (104%)	424 (95%)	24 (5%)	22	20
All	All	896/858 (104%)	848 (95%)	48 (5%)	22	20

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	47	LEU
1	A	87	LEU
1	A	112	GLU
1	A	221	ASP
1	A	262	ARG
1	A	280	ARG
1	A	281	TRP
1	A	284	ARG
1	A	289	LEU
1	A	307	GLN
1	A	347	GLU
1	A	351	SER
1	A	367	ASN
1	A	393	ILE

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Mol	Chain	Res	Type
1	A	398	ILE
1	A	447	TYR
1	A	480	ARG
1	A	481	GLN
1	A	486	PHE
1	A	489	ASP
1	A	501	SER
1	A	556	GLU
1	A	557	ARG
1	B	3	ARG
1	B	7	VAL
1	B	111	LYS
1	B	113	ASP
1	B	131	VAL
1	B	254	MSE
1	B	258	GLN
1	B	261	GLN
1	B	262	ARG
1	B	263	TYR
1	B	269	LEU
1	B	292	TYR
1	B	306	THR
1	B	386	ASP
1	B	393	ILE
1	B	396	SER
1	B	398	ILE
1	B	402	GLN
1	B	447	TYR
1	B	464	LEU
1	B	478	LEU
1	B	481	GLN
1	B	487	ASP
1	B	542	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 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	539/558 (96%)	0.41	52 (9%)	8	10	28, 41, 139, 232	0
1	B	539/558 (96%)	0.82	62 (11%)	4	6	28, 42, 132, 200	0
All	All	1078/1116 (96%)	0.61	114 (10%)	6	7	28, 41, 133, 232	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	287	GLY	23.3
1	A	287	GLY	19.7
1	B	264	GLY	17.4
1	B	263	TYR	15.9
1	B	558	VAL	15.4
1	B	289	LEU	14.7
1	B	286	THR	14.5
1	B	399	ALA	13.2
1	B	306	THR	12.1
1	A	289	LEU	10.7
1	B	307	GLN	10.6
1	A	286	THR	10.4
1	A	259	THR	10.3
1	B	262	ARG	10.2
1	B	398	ILE	10.2
1	B	401	GLY	10.2
1	A	262	ARG	10.1
1	A	399	ALA	10.0
1	B	402	GLN	9.8
1	A	306	THR	9.7
1	B	288	GLY	9.6
1	B	285	HIS	9.6
1	A	288	GLY	9.4
1	A	398	ILE	9.3

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Mol	Chain	Res	Type	RSRZ
1	B	260	SER	9.0
1	B	305	PRO	8.6
1	A	114	PHE	8.4
1	B	290	ASP	8.2
1	B	312	PHE	8.0
1	B	261	GLN	7.9
1	A	483	GLN	7.9
1	A	283	ASN	7.9
1	B	284	ARG	7.9
1	B	259	THR	7.8
1	B	478	LEU	7.8
1	A	263	TYR	7.7
1	A	257	LEU	7.7
1	A	480	ARG	7.5
1	A	558	VAL	7.4
1	A	401	GLY	7.2
1	B	256	GLY	7.1
1	B	482	SER	6.9
1	A	110	TYR	6.9
1	B	291	VAL	6.8
1	B	395	LEU	6.8
1	B	257	LEU	6.6
1	A	261	GLN	6.3
1	B	394	GLY	6.3
1	B	486	PHE	6.0
1	A	108	ARG	6.0
1	B	292	TYR	5.8
1	B	484	ARG	5.8
1	B	294	GLU	5.7
1	A	311	VAL	5.6
1	B	483	GLN	5.6
1	A	312	PHE	5.3
1	A	362	LYS	5.1
1	B	2	PRO	5.0
1	B	485	GLY	4.9
1	A	400	GLY	4.9
1	A	479	ILE	4.9
1	B	111	LYS	4.9
1	A	305	PRO	4.7
1	A	481	GLN	4.7
1	A	307	GLN	4.6
1	A	482	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	361	ARG	4.6
1	B	479	ILE	4.5
1	B	110	TYR	4.5
1	A	258	GLN	4.3
1	A	395	LEU	4.3
1	A	285	HIS	4.3
1	B	361	ARG	4.3
1	A	282	ALA	4.3
1	B	258	GLN	4.2
1	B	283	ASN	4.1
1	B	480	ARG	4.0
1	A	111	LYS	3.9
1	B	397	GLN	3.9
1	B	282	ALA	3.8
1	B	362	LYS	3.7
1	B	308	ILE	3.6
1	B	113	ASP	3.6
1	B	112	GLU	3.6
1	A	484	ARG	3.6
1	B	293	THR	3.5
1	B	557	ARG	3.5
1	B	481	GLN	3.5
1	B	114	PHE	3.4
1	A	113	ASP	3.3
1	A	292	TYR	3.2
1	A	363	THR	3.1
1	A	112	GLU	3.1
1	A	486	PHE	3.1
1	A	397	GLN	3.0
1	B	363	THR	3.0
1	A	284	ARG	2.9
1	A	310	ARG	2.8
1	B	255	VAL	2.7
1	B	357	ARG	2.7
1	B	108	ARG	2.6
1	A	294	GLU	2.5
1	B	268	LEU	2.5
1	B	396	SER	2.5
1	A	107	ALA	2.5
1	A	308	ILE	2.4
1	B	296	ARG	2.3
1	A	260	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	400	GLY	2.2
1	A	293	THR	2.2
1	A	417	GLN	2.2
1	A	478	LEU	2.1
1	B	107	ALA	2.1
1	A	2	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.