WORLDWIDE
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2025 – 02:42 PM JST

PDB ID	:	9II8 / pdb_00009ii8
Title	:	Crystal structure of Staphylococcus aureus DinG protein in complex with ss-DNA
Authors	:	Cheng, K.
Deposited on	:	2024-06-19
Resolution	:	3.16 Å(reported)

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

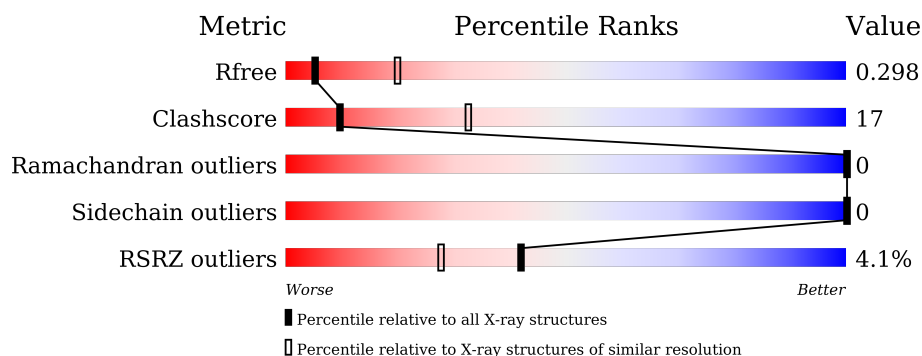|		
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 3.16 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 — 0.298
Clashscore — 17
Ramachandran outliers — 0
Sidechain outliers — 0
RSRZ outliers — 4.1%

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}	164625	2168 (3.20-3.12)
Clashscore	180529	2333 (3.20-3.12)
Ramachandran outliers	177936	2266 (3.20-3.12)
Sidechain outliers	177891	2265 (3.20-3.12)
RSRZ outliers	164620	2169 (3.20-3.12)

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	B	4	75% 25%
2	A	897	4% 68% 32% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7432 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 DNA chain called DNA (5'-D(P*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	4	Total 80	C 40	N 8	O 28	P 4	0	0	0

- Molecule 2 is a protein called 3'-5' exonuclease DinG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	896	Total 7352	C 4739	N 1207	O 1380	S 26	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	210	PHE	SER	conflict	UNP Q2FYH5
A	241	ARG	SER	conflict	UNP Q2FYH5

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.
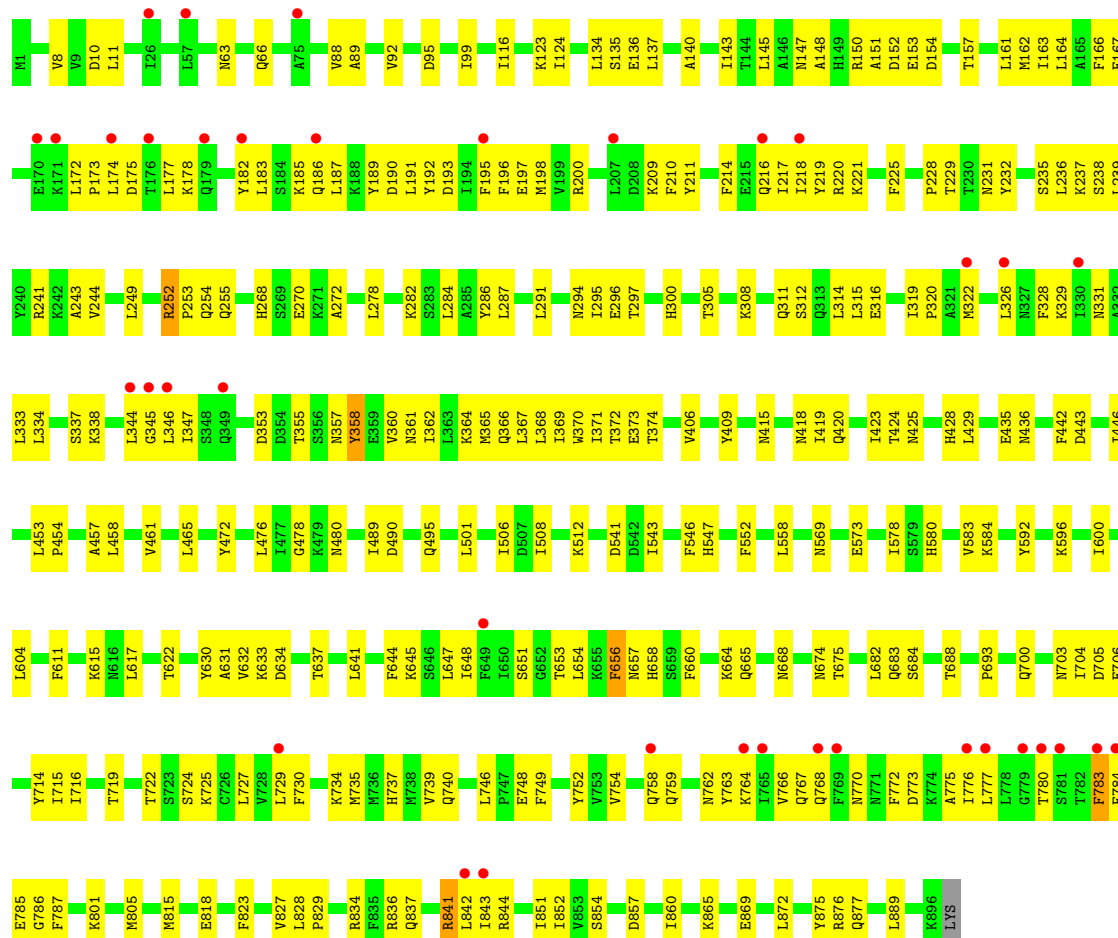
• Molecule 1: DNA (5'-D(P*TP*TP*TP*T)-3')

Chain B:

75%   25%

• Molecule 2: 3'-5' exonuclease DinG

Chain A:

4%

68%   32%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	229.17Å 229.17Å 128.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	111.77 – 3.16 111.77 – 3.16	Depositor EDS
% Data completeness (in resolution range)	100.0 (111.77-3.16) 99.9 (111.77-3.16)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.269 , 0.293 0.272 , 0.298	Depositor DCC
R_{free} test set	1482 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	115.6	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 86.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7432	wwPDB-VP
Average B, all atoms (Å^2)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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 (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	B	0.60	0/87	1.03	0/132
2	A	0.83	0/7495	1.05	6/10110 (0.1%)
All	All	0.83	0/7582	1.05	6/10242 (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
2	A	0	6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	478	GLY	CA-C-O	-6.36	118.09	122.22
2	A	358	TYR	N-CA-CB	-5.77	101.41	110.06
2	A	783	PHE	CA-CB-CG	5.38	119.18	113.80
2	A	656	PHE	N-CA-C	-5.27	102.66	110.46
2	A	345	GLY	N-CA-C	-5.18	108.88	115.31
2	A	305	THR	CA-CB-OG1	-5.18	101.83	109.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	252	ARG	Sidechain
2	A	834	ARG	Sidechain
2	A	836	ARG	Sidechain
2	A	841	ARG	Sidechain
2	A	844	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	A	876	ARG	Sidechain

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	B	80	0	49	2	0
2	A	7352	0	7397	259	1
All	All	7432	0	7446	259	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 17.

All (259) 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)
2:A:772:PHE:CB	2:A:776:ILE:HD11	1.53	1.37
2:A:772:PHE:HB3	2:A:776:ILE:CD1	1.64	1.25
2:A:369:ILE:O	2:A:372:THR:HG22	1.40	1.20
2:A:775:ALA:O	2:A:776:ILE:CD1	1.90	1.19
2:A:344:LEU:HD23	2:A:406:VAL:HG13	1.31	1.12
2:A:775:ALA:O	2:A:776:ILE:HD13	0.96	1.12
2:A:88:VAL:HG11	2:A:162:MET:HE2	1.33	1.08
2:A:823:PHE:HA	2:A:827:VAL:HG22	1.38	1.06
2:A:237:LYS:H	2:A:237:LYS:HD2	0.96	1.06
2:A:252:ARG:HH12	2:A:682:LEU:HD12	1.17	1.04
2:A:192:TYR:CD2	2:A:193:ASP:OD1	2.12	1.02
2:A:252:ARG:NH1	2:A:682:LEU:HD12	1.74	1.02
2:A:192:TYR:CE2	2:A:193:ASP:OD1	2.13	1.01
2:A:775:ALA:C	2:A:776:ILE:HD13	1.84	1.01
2:A:88:VAL:HG11	2:A:162:MET:CE	1.96	0.96
2:A:443:ASP:HB3	2:A:645:LYS:HG2	1.48	0.95
2:A:237:LYS:H	2:A:237:LYS:CD	1.79	0.94
2:A:724:SER:O	2:A:752:TYR:OH	1.83	0.94
2:A:660:PHE:CE2	2:A:675:THR:OG1	2.21	0.94
2:A:237:LYS:HD2	2:A:237:LYS:N	1.81	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:300:HIS:HA	2:A:420:GLN:HA	1.54	0.89
2:A:727:LEU:HD11	2:A:783:PHE:HZ	1.35	0.89
2:A:772:PHE:O	2:A:776:ILE:HG12	1.73	0.88
2:A:727:LEU:HD11	2:A:783:PHE:CZ	2.09	0.87
2:A:229:THR:HA	2:A:328:PHE:CD1	2.13	0.84
2:A:424:THR:HG22	2:A:425:ASN:H	1.44	0.82
2:A:229:THR:HA	2:A:328:PHE:CE1	2.16	0.81
1:B:5:DT:O3'	2:A:734:LYS:HE3	1.83	0.79
2:A:641:LEU:HA	2:A:647:LEU:CD1	2.16	0.75
2:A:752:TYR:HA	2:A:775:ALA:HB1	1.67	0.75
2:A:785:GLU:HB3	2:A:837:GLN:HG2	1.68	0.73
2:A:780:THR:HG21	2:A:783:PHE:CD1	2.14	0.73
2:A:192:TYR:HE2	2:A:193:ASP:OD1	1.71	0.73
2:A:637:THR:HG21	2:A:668:ASN:H	1.54	0.72
2:A:490:ASP:HB2	2:A:508:ILE:CD1	2.19	0.72
2:A:842:LEU:HD22	2:A:852:ILE:HG13	1.70	0.72
2:A:344:LEU:CD2	2:A:406:VAL:HG13	2.17	0.72
2:A:192:TYR:HD2	2:A:193:ASP:OD1	1.69	0.72
2:A:210:PHE:HD1	2:A:219:TYR:O	1.73	0.72
2:A:11:LEU:HD11	2:A:99:ILE:HG13	1.72	0.70
2:A:369:ILE:O	2:A:372:THR:CG2	2.31	0.70
2:A:580:HIS:HB3	2:A:583:VAL:HG12	1.74	0.69
2:A:746:LEU:HB3	2:A:748:GLU:OE2	1.93	0.69
2:A:358:TYR:CE1	2:A:362:ILE:HD11	2.29	0.68
2:A:252:ARG:NH1	2:A:682:LEU:CD1	2.55	0.68
2:A:311:GLN:HG3	2:A:423:ILE:HD12	1.76	0.67
2:A:315:LEU:HD22	2:A:423:ILE:HD11	1.76	0.67
2:A:239:LEU:HD21	2:A:291:LEU:HD11	1.76	0.67
2:A:346:LEU:HD11	2:A:367:LEU:HB3	1.77	0.67
2:A:137:LEU:O	2:A:140:ALA:HB3	1.95	0.67
2:A:772:PHE:HB3	2:A:776:ILE:HD11	0.73	0.67
2:A:353:ASP:O	2:A:353:ASP:OD2	2.12	0.67
2:A:633:LYS:HD2	2:A:818:GLU:HG2	1.76	0.67
2:A:143:ILE:HD11	2:A:164:LEU:HD11	1.77	0.66
2:A:161:LEU:HD23	2:A:164:LEU:HD12	1.78	0.66
2:A:210:PHE:HD1	2:A:219:TYR:C	2.04	0.66
2:A:490:ASP:CA	2:A:508:ILE:HD12	2.26	0.65
2:A:823:PHE:HA	2:A:827:VAL:CG2	2.22	0.64
2:A:322:MET:HE2	2:A:322:MET:HA	1.79	0.64
2:A:703:ASN:HB3	2:A:706:GLU:OE1	1.97	0.64
2:A:752:TYR:CD1	2:A:777:LEU:HG	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:209:LYS:H	2:A:209:LYS:HD2	1.61	0.64
2:A:197:GLU:HA	2:A:200:ARG:HD3	1.80	0.64
2:A:641:LEU:HA	2:A:647:LEU:HD11	1.78	0.64
2:A:236:LEU:HD23	2:A:237:LYS:NZ	2.13	0.63
2:A:727:LEU:CD1	2:A:783:PHE:HZ	2.08	0.63
1:B:5:DT:O3'	2:A:734:LYS:CE	2.47	0.63
2:A:235:SER:HB2	2:A:237:LYS:NZ	2.13	0.63
2:A:780:THR:CG2	2:A:783:PHE:CD1	2.60	0.63
2:A:124:ILE:HD11	2:A:186:GLN:HE22	1.64	0.62
2:A:446:ILE:HG22	2:A:648:ILE:HB	1.81	0.62
2:A:163:ILE:O	2:A:167:GLU:HG3	2.00	0.61
2:A:558:LEU:HD21	2:A:604:LEU:HB2	1.81	0.61
2:A:116:ILE:HG23	2:A:191:LEU:HD21	1.82	0.61
2:A:145:LEU:HD13	2:A:145:LEU:O	2.01	0.61
2:A:235:SER:HB2	2:A:237:LYS:HZ2	1.66	0.61
2:A:135:SER:HA	2:A:145:LEU:HG	1.81	0.61
2:A:490:ASP:CB	2:A:508:ILE:HD12	2.30	0.61
2:A:361:ASN:HA	2:A:364:LYS:HD2	1.83	0.60
2:A:428:HIS:O	2:A:436:ASN:ND2	2.35	0.60
2:A:490:ASP:CB	2:A:508:ILE:CD1	2.80	0.60
2:A:88:VAL:CG1	2:A:162:MET:HE2	2.23	0.59
2:A:337:SER:HB3	2:A:435:GLU:HG2	1.82	0.59
2:A:641:LEU:HA	2:A:647:LEU:HD12	1.85	0.59
2:A:235:SER:OG	2:A:237:LYS:HD3	2.03	0.59
2:A:631:ALA:HB3	2:A:634:ASP:HB2	1.84	0.59
2:A:786:GLY:H	2:A:841:ARG:NH2	2.00	0.59
2:A:700:GLN:HE21	2:A:703:ASN:HB2	1.68	0.58
2:A:490:ASP:HB2	2:A:508:ILE:HD12	1.84	0.58
2:A:716:ILE:HD11	2:A:746:LEU:HD13	1.84	0.58
2:A:252:ARG:HD2	2:A:253:PRO:HD2	1.84	0.58
2:A:424:THR:HG22	2:A:425:ASN:N	2.17	0.58
2:A:236:LEU:HD23	2:A:237:LYS:CE	2.33	0.57
2:A:172:LEU:HB2	2:A:175:ASP:OD2	2.05	0.57
2:A:344:LEU:HD23	2:A:406:VAL:CG1	2.22	0.57
2:A:543:ILE:HG13	2:A:759:GLN:HG3	1.87	0.57
2:A:210:PHE:CD1	2:A:219:TYR:C	2.84	0.56
2:A:828:LEU:HB3	2:A:829:PRO:HD3	1.87	0.56
2:A:232:TYR:HE2	2:A:238:SER:HB2	1.70	0.56
2:A:490:ASP:HA	2:A:508:ILE:HD12	1.86	0.56
2:A:150:ARG:HD3	2:A:152:ASP:HB2	1.87	0.56
2:A:8:VAL:HG22	2:A:162:MET:CE	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:211:TYR:HB3	2:A:221:LYS:HD2	1.87	0.56
2:A:429:LEU:HD11	2:A:644:PHE:HE2	1.72	0.55
2:A:719:THR:HG22	2:A:752:TYR:CZ	2.42	0.55
2:A:89:ALA:HB3	2:A:92:VAL:HG23	1.88	0.55
2:A:255:GLN:HA	2:A:278:LEU:HD11	1.87	0.55
2:A:228:PRO:O	2:A:328:PHE:HD1	1.91	0.54
2:A:186:GLN:NE2	2:A:365:MET:SD	2.80	0.54
2:A:453:LEU:N	2:A:454:PRO:HD2	2.22	0.54
2:A:123:LYS:HB3	2:A:366:GLN:HE21	1.72	0.54
2:A:458:LEU:O	2:A:461:VAL:HG12	2.07	0.54
2:A:150:ARG:HD2	2:A:153:GLU:HG2	1.90	0.54
2:A:210:PHE:CD1	2:A:220:ARG:HA	2.44	0.53
2:A:780:THR:HG21	2:A:783:PHE:CZ	2.24	0.53
2:A:730:PHE:CZ	2:A:739:VAL:HG11	2.44	0.53
2:A:214:PHE:CD2	2:A:344:LEU:HB3	2.44	0.53
2:A:185:LYS:HD3	2:A:355:THR:HB	1.90	0.52
2:A:172:LEU:HD23	2:A:218:ILE:HD13	1.91	0.52
2:A:192:TYR:CD2	2:A:193:ASP:N	2.78	0.52
2:A:772:PHE:CB	2:A:776:ILE:CD1	2.49	0.52
2:A:872:LEU:O	2:A:877:GLN:NE2	2.40	0.52
2:A:329:LYS:HZ2	2:A:331:ASN:HA	1.75	0.52
2:A:254:GLN:HE21	2:A:254:GLN:HA	1.75	0.52
2:A:210:PHE:CD1	2:A:219:TYR:O	2.59	0.51
2:A:175:ASP:OD2	2:A:218:ILE:HD13	2.10	0.51
2:A:569:ASN:O	2:A:573:GLU:HG2	2.10	0.51
2:A:166:PHE:N	2:A:166:PHE:CD1	2.76	0.51
2:A:315:LEU:HD22	2:A:423:ILE:CD1	2.40	0.51
2:A:63:ASN:HA	2:A:66:GLN:NE2	2.27	0.50
2:A:236:LEU:HD23	2:A:237:LYS:HZ2	1.75	0.50
2:A:174:LEU:HA	2:A:177:LEU:HD12	1.94	0.50
2:A:244:VAL:HG23	2:A:249:LEU:HB2	1.92	0.50
2:A:415:ASN:O	2:A:419:ILE:HG12	2.12	0.50
2:A:637:THR:CG2	2:A:668:ASN:H	2.21	0.50
2:A:752:TYR:HD1	2:A:777:LEU:HG	1.74	0.50
2:A:552:PHE:HE1	2:A:611:PHE:HA	1.76	0.49
2:A:615:LYS:HB3	2:A:622:THR:HB	1.93	0.49
2:A:805:MET:SD	2:A:827:VAL:HG12	2.51	0.49
2:A:369:ILE:C	2:A:372:THR:HG22	2.31	0.49
2:A:633:LYS:NZ	2:A:665:GLN:O	2.41	0.49
2:A:872:LEU:HB3	2:A:877:GLN:HE21	1.78	0.49
2:A:8:VAL:HG22	2:A:162:MET:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:592:TYR:CE2	2:A:596:LYS:HE2	2.47	0.49
2:A:228:PRO:O	2:A:328:PHE:CD1	2.65	0.48
2:A:145:LEU:HA	2:A:157:THR:HG21	1.95	0.48
2:A:368:LEU:O	2:A:371:ILE:HG22	2.14	0.48
2:A:683:GLN:O	2:A:684:SER:C	2.57	0.48
2:A:291:LEU:HD13	2:A:326:LEU:HD21	1.95	0.48
2:A:768:GLN:HG3	2:A:776:ILE:HG21	1.95	0.48
2:A:182:TYR:CE1	2:A:364:LYS:HD3	2.49	0.47
2:A:252:ARG:CZ	2:A:682:LEU:HD12	2.42	0.47
2:A:195:PHE:HA	2:A:198:MET:HE2	1.97	0.47
2:A:358:TYR:HE1	2:A:362:ILE:HD11	1.77	0.47
2:A:752:TYR:CE1	2:A:777:LEU:HG	2.50	0.47
2:A:786:GLY:H	2:A:841:ARG:CZ	2.27	0.47
2:A:851:ILE:HD13	2:A:889:LEU:HD21	1.96	0.47
2:A:767:GLN:HA	2:A:770:ASN:HB2	1.96	0.47
2:A:187:LEU:HD23	2:A:189:TYR:CE2	2.48	0.47
2:A:715:ILE:O	2:A:719:THR:OG1	2.22	0.47
2:A:722:THR:HG23	2:A:722:THR:O	2.13	0.47
2:A:703:ASN:O	2:A:706:GLU:OE1	2.33	0.47
2:A:704:ILE:HD11	2:A:735:MET:HB2	1.96	0.47
2:A:178:LYS:HE2	2:A:216:GLN:HG3	1.96	0.47
2:A:578:ILE:HG12	2:A:583:VAL:HG11	1.97	0.47
2:A:272:ALA:HA	2:A:674:ASN:H	1.79	0.47
2:A:693:PRO:HB3	2:A:714:TYR:OH	2.15	0.46
2:A:656:PHE:O	2:A:657:ASN:C	2.56	0.46
2:A:150:ARG:O	2:A:154:ASP:HB2	2.15	0.46
2:A:660:PHE:CZ	2:A:675:THR:OG1	2.66	0.46
2:A:865:LYS:O	2:A:869:GLU:HG2	2.15	0.46
2:A:147:ASN:HB3	2:A:150:ARG:HE	1.80	0.46
2:A:372:THR:HG23	2:A:373:GLU:HG3	1.96	0.46
2:A:231:ASN:HA	2:A:295:ILE:HG23	1.97	0.46
2:A:490:ASP:HB2	2:A:508:ILE:HD11	1.96	0.46
2:A:787:PHE:O	2:A:841:ARG:HD2	2.16	0.46
2:A:153:GLU:O	2:A:157:THR:N	2.43	0.46
2:A:754:VAL:HG12	2:A:777:LEU:HD12	1.97	0.46
2:A:10:ASP:OD2	2:A:151:ALA:HA	2.15	0.45
2:A:236:LEU:HD23	2:A:237:LYS:HD2	1.98	0.45
2:A:217:ILE:HD13	2:A:346:LEU:HB3	1.99	0.45
2:A:547:HIS:HB2	2:A:617:LEU:HD11	1.99	0.45
2:A:651:SER:HB3	2:A:654:LEU:HG	1.99	0.45
2:A:190:ASP:OD1	2:A:192:TYR:OH	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:657:ASN:HB3	2:A:658:HIS:H	1.60	0.44
2:A:801:LYS:HB3	2:A:801:LYS:HE3	1.66	0.44
2:A:236:LEU:CD2	2:A:237:LYS:NZ	2.78	0.44
2:A:495:GLN:HB3	2:A:501:LEU:HG	1.99	0.44
2:A:134:LEU:CD2	2:A:154:ASP:HA	2.46	0.44
2:A:145:LEU:HD13	2:A:145:LEU:C	2.43	0.44
2:A:282:LYS:HB3	2:A:286:TYR:CZ	2.51	0.44
2:A:472:TYR:CE2	2:A:476:LEU:HD11	2.52	0.44
2:A:370:TRP:NE1	2:A:374:THR:HB	2.33	0.44
2:A:300:HIS:HB2	2:A:442:PHE:CE2	2.53	0.44
2:A:857:ASP:O	2:A:860:ILE:HG12	2.18	0.44
2:A:705:ASP:OD1	2:A:706:GLU:OE1	2.35	0.44
2:A:8:VAL:HG22	2:A:162:MET:HE3	2.00	0.44
2:A:196:PHE:CE2	2:A:200:ARG:HD2	2.53	0.44
2:A:357:ASN:HB3	2:A:360:VAL:HG23	2.00	0.43
2:A:785:GLU:HB3	2:A:837:GLN:CG	2.43	0.43
2:A:758:GLN:HE22	2:A:764:LYS:HG3	1.84	0.43
2:A:780:THR:HB	2:A:783:PHE:HD1	1.31	0.43
2:A:225:PHE:HE2	2:A:333:LEU:HD12	1.84	0.43
2:A:461:VAL:HG22	2:A:630:TYR:O	2.18	0.43
2:A:465:LEU:HB2	2:A:600:ILE:HG13	2.01	0.43
2:A:268:HIS:HB2	2:A:270:GLU:HG3	2.01	0.43
2:A:763:TYR:O	2:A:766:VAL:HG22	2.19	0.43
2:A:775:ALA:C	2:A:776:ILE:CD1	2.72	0.43
2:A:136:GLU:O	2:A:140:ALA:HB2	2.18	0.42
2:A:284:LEU:HD12	2:A:287:LEU:HD11	2.01	0.42
2:A:11:LEU:HD12	2:A:95:ASP:HA	2.01	0.42
2:A:338:LYS:HA	2:A:409:TYR:CD1	2.55	0.42
2:A:489:ILE:HG23	2:A:506:ILE:HG21	2.01	0.42
2:A:653:THR:O	2:A:653:THR:OG1	2.32	0.42
2:A:183:LEU:HG	2:A:365:MET:HE1	2.00	0.42
2:A:319:ILE:HB	2:A:320:PRO:HD3	2.02	0.42
2:A:648:ILE:O	2:A:648:ILE:HG22	2.18	0.42
2:A:134:LEU:HD21	2:A:157:THR:OG1	2.20	0.42
2:A:153:GLU:O	2:A:157:THR:OG1	2.37	0.42
2:A:729:LEU:HB3	2:A:784:PHE:CE1	2.55	0.42
2:A:145:LEU:HD11	2:A:148:ALA:HB2	2.01	0.42
2:A:547:HIS:CB	2:A:617:LEU:HD11	2.49	0.42
2:A:725:LYS:HE2	2:A:773:ASP:HA	2.02	0.42
2:A:737:HIS:HA	2:A:740:GLN:HG2	2.02	0.42
2:A:185:LYS:HD3	2:A:355:THR:CB	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:334:LEU:HA	2:A:423:ILE:HG12	2.02	0.41
2:A:243:ALA:HB1	2:A:322:MET:HE1	2.01	0.41
2:A:291:LEU:O	2:A:294:ASN:HB3	2.20	0.41
2:A:584:LYS:HE3	2:A:584:LYS:HB2	1.94	0.41
2:A:300:HIS:ND1	2:A:442:PHE:HA	2.35	0.41
2:A:217:ILE:HD11	2:A:347:ILE:N	2.36	0.41
2:A:480:ASN:HA	2:A:512:LYS:HE3	2.02	0.41
2:A:664:LYS:HE3	2:A:664:LYS:HB2	1.83	0.41
2:A:693:PRO:HD2	2:A:854:SER:O	2.21	0.41
2:A:429:LEU:HD11	2:A:644:PHE:CE2	2.55	0.41
2:A:682:LEU:HB3	2:A:683:GLN:H	1.61	0.41
2:A:725:LYS:CE	2:A:773:ASP:HA	2.50	0.41
2:A:284:LEU:O	2:A:287:LEU:HG	2.21	0.41
2:A:637:THR:HG21	2:A:668:ASN:N	2.31	0.41
2:A:172:LEU:HD23	2:A:218:ILE:CD1	2.51	0.41
2:A:173:PRO:O	2:A:174:LEU:C	2.64	0.41
2:A:312:SER:O	2:A:316:GLU:HG2	2.20	0.41
2:A:746:LEU:HB2	2:A:749:PHE:HD2	1.86	0.41
2:A:758:GLN:NE2	2:A:762:ASN:HA	2.36	0.41
2:A:541:ASP:CG	2:A:546:PHE:H	2.29	0.41
2:A:314:LEU:O	2:A:319:ILE:HG12	2.22	0.40
2:A:329:LYS:NZ	2:A:331:ASN:HA	2.36	0.40
2:A:331:ASN:HD21	2:A:418:ASN:C	2.29	0.40
2:A:453:LEU:HD12	2:A:453:LEU:HA	1.91	0.40
2:A:457:ALA:O	2:A:461:VAL:HB	2.21	0.40
2:A:688:THR:OG1	2:A:875:TYR:CE1	2.73	0.40
2:A:684:SER:HB3	2:A:843:ILE:HG21	2.03	0.40
2:A:153:GLU:OE1	2:A:157:THR:HG23	2.21	0.40
2:A:308:LYS:O	2:A:311:GLN:HB3	2.22	0.40
2:A:183:LEU:HD22	2:A:191:LEU:HB2	2.03	0.40
2:A:333:LEU:HD23	2:A:334:LEU:N	2.36	0.40
2:A:296:GLU:O	2:A:297:THR:C	2.64	0.40
2:A:632:VAL:HG21	2:A:815:MET:SD	2.62	0.40
2:A:693:PRO:HB3	2:A:714:TYR:CZ	2.56	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)
2:A:66:GLN:NE2	2:A:241:ARG:CD[4_555]	1.96	0.24

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	
2	A	894/897 (100%)	846 (95%)	48 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	A	819/820 (100%)	819 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	17	GLN
2	A	34	ASN
2	A	76	GLN
2	A	186	GLN
2	A	216	GLN
2	A	233	ASN
2	A	254	GLN
2	A	255	GLN
2	A	294	ASN
2	A	366	GLN
2	A	431	HIS

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Mol	Chain	Res	Type
2	A	674	ASN
2	A	700	GLN
2	A	737	HIS
2	A	744	ASN
2	A	767	GLN
2	A	770	ASN
2	A	845	ASN
2	A	891	GLN
2	A	893	GLN

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 oligosaccharides 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(Å²)	Q<0.9
1	B	4/4 (100%)	0.61	0	100	100	116, 119, 142, 143	0
2	A	896/897 (99%)	0.32	37 (4%)	42	28	55, 113, 184, 212	0
All	All	900/901 (99%)	0.32	37 (4%)	42	28	55, 113, 184, 212	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	780	THR	5.8
2	A	182	TYR	4.7
2	A	322	MET	3.9
2	A	768	GLN	3.9
2	A	349	GLN	3.5
2	A	179	GLN	3.5
2	A	345	GLY	3.4
2	A	783	PHE	3.2
2	A	784	PHE	3.2
2	A	326	LEU	3.0
2	A	776	ILE	3.0
2	A	186	GLN	2.9
2	A	842	LEU	2.8
2	A	764	LYS	2.8
2	A	330	ILE	2.8
2	A	729	LEU	2.7
2	A	765	ILE	2.6
2	A	26	ILE	2.6
2	A	75	ALA	2.6
2	A	218	ILE	2.5
2	A	344	LEU	2.4
2	A	346	LEU	2.4
2	A	649	PHE	2.4
2	A	207	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	170	GLU	2.3
2	A	174	LEU	2.3
2	A	777	LEU	2.3
2	A	843	ILE	2.3
2	A	195	PHE	2.3
2	A	758	GLN	2.3
2	A	779	GLY	2.1
2	A	216	GLN	2.1
2	A	57	LEU	2.1
2	A	176	THR	2.1
2	A	769	PHE	2.0
2	A	781	SER	2.0
2	A	171	LYS	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 oligosaccharides 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.