



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:06 AM UTC

PDB ID : 2Z2O / pdb_00002z2o
Title : Crystal Structure of apo virginiamycin B lyase from Staphylococcus aureus
Authors : Korczynska, M.; Berghuis, A.M.
Deposited on : 2007-05-25
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

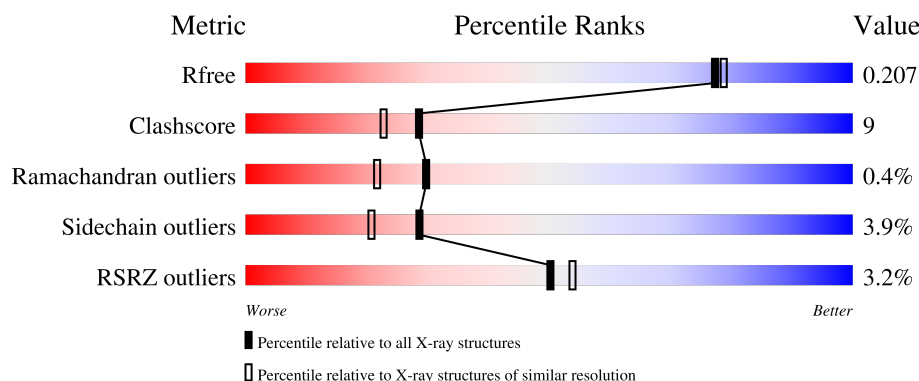
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	299	4% 82% 16% .
1	B	299	3% 77% 19% ..
1	C	299	4% 80% 18% .
1	D	299	2% 81% 16% ...

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	D	301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10412 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 virginiamycin B lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	8	0
			2346	1495	386	454	11			
1	B	293	Total	C	N	O	S	0	8	0
			2311	1471	381	449	10			
1	C	299	Total	C	N	O	S	0	5	0
			2344	1488	385	460	11			
1	D	295	Total	C	N	O	S	1	6	0
			2323	1479	383	449	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	THR	PRO	SEE REMARK 999	UNP Q53744
A	212	SER	LEU	SEE REMARK 999	UNP Q53744
B	211	THR	PRO	SEE REMARK 999	UNP Q53744
B	212	SER	LEU	SEE REMARK 999	UNP Q53744
C	211	THR	PRO	SEE REMARK 999	UNP Q53744
C	212	SER	LEU	SEE REMARK 999	UNP Q53744
D	211	THR	PRO	SEE REMARK 999	UNP Q53744
D	212	SER	LEU	SEE REMARK 999	UNP Q53744

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		
2	D	2	Total	Cl	0	0
			2	2		

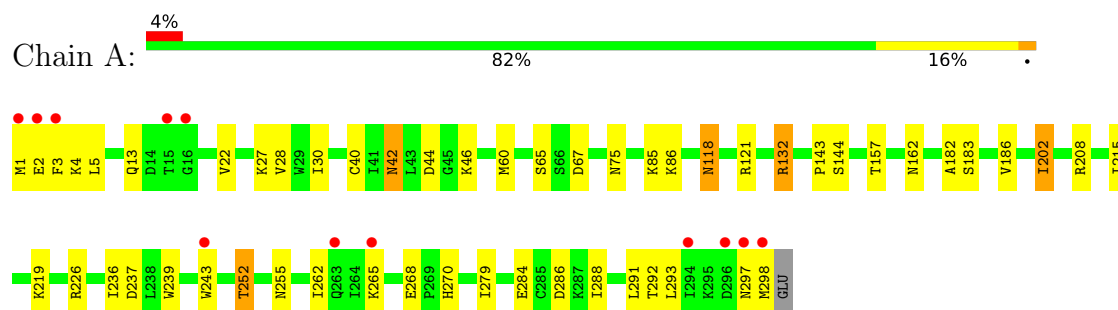
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	327	Total 327	O 327	0	0
3	B	290	Total 290	O 290	0	0
3	C	232	Total 232	O 232	0	0
3	D	234	Total 234	O 234	0	0

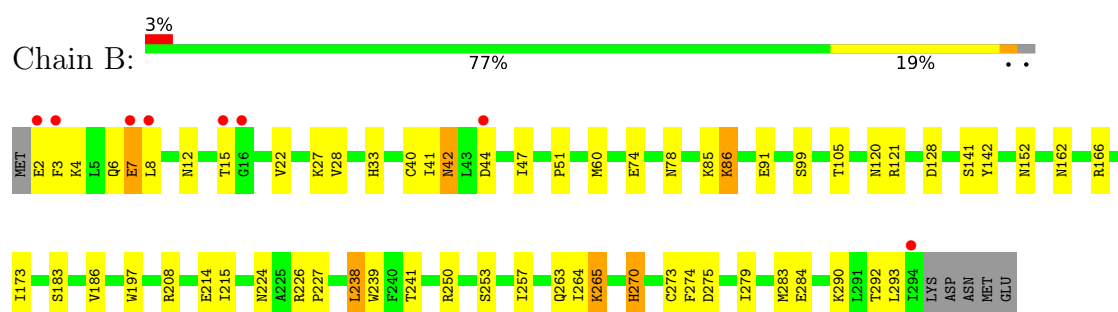
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

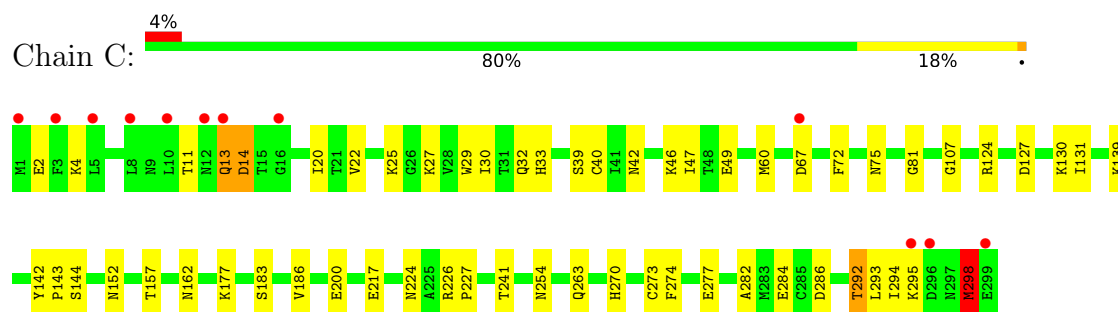
• Molecule 1: virginiamycin B lyase



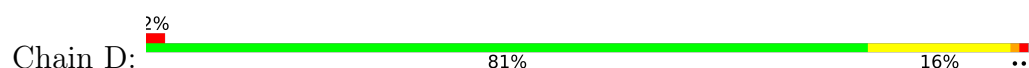
• Molecule 1: virginiamycin B lyase

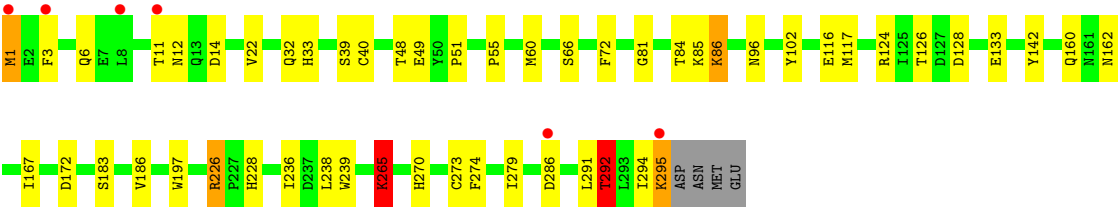


• Molecule 1: virginiamycin B lyase



• Molecule 1: virginiamycin B lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.54Å 79.23Å 188.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 1.90 19.89 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.89-1.90) 99.6 (19.89-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.140 , 0.199 0.154 , 0.207	Depositor DCC
R_{free} test set	8108 reflections (9.29%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10412	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.28	3/2424 (0.1%)	1.08	4/3293 (0.1%)
1	B	1.20	5/2389 (0.2%)	1.05	2/3248 (0.1%)
1	C	1.20	3/2413 (0.1%)	1.04	3/3276 (0.1%)
1	D	1.17	3/2392 (0.1%)	1.08	6/3248 (0.2%)
All	All	1.21	14/9618 (0.1%)	1.06	15/13065 (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	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	ARG	CB-CG	-7.47	1.30	1.52
1	C	142	TYR	N-CA	7.16	1.51	1.46
1	D	270	HIS	CA-C	6.85	1.55	1.52
1	B	142	TYR	C-O	6.69	1.27	1.23
1	D	160	GLN	C-O	-5.97	1.15	1.24
1	B	270	HIS	CA-C	5.48	1.55	1.52
1	B	121	ARG	CB-CG	-5.35	1.36	1.52
1	C	131	ILE	N-CA	5.33	1.52	1.46
1	A	121	ARG	CB-CG	-5.29	1.36	1.52
1	C	282	ALA	C-O	-5.25	1.17	1.24
1	B	105	THR	C-O	-5.20	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	TYR	N-CA	5.19	1.50	1.46
1	D	228	HIS	CA-C	5.13	1.56	1.52
1	A	182	ALA	CA-CB	-5.07	1.45	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	PHE	N-CA-C	8.40	121.48	108.96
1	D	226	ARG	CB-CA-C	-7.78	104.23	111.00
1	D	265	LYS	CA-C-O	7.66	129.73	120.92
1	D	66	SER	CA-C-N	-6.49	112.84	122.83
1	D	66	SER	C-N-CA	-6.49	112.84	122.83
1	D	292	THR	N-CA-C	6.41	118.86	108.34
1	C	107	GLY	CA-C-N	6.37	126.29	119.28
1	C	107	GLY	C-N-CA	6.37	126.29	119.28
1	B	152	ASN	N-CA-C	6.11	120.32	112.86
1	A	202	ILE	CB-CA-C	-5.90	104.20	111.92
1	D	124	ARG	N-CA-CB	-5.41	101.72	110.81
1	A	262	ILE	N-CA-C	-5.22	100.93	108.71
1	A	132	ARG	N-CA-CB	-5.19	101.60	111.00
1	B	238	LEU	CA-CB-CG	-5.06	98.59	116.30
1	C	263	GLN	CA-CB-CG	-5.01	104.08	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	GLU	Peptide
1	C	298	MET	Peptide
1	D	294	ILE	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2346	0	2334	41	0
1	B	2311	0	2290	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2344	0	2312	35	0
1	D	2323	0	2304	41	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	2	0
3	A	327	0	0	7	0
3	B	290	0	0	11	0
3	C	232	0	0	7	0
3	D	234	0	0	10	0
All	All	10412	0	9240	164	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 9.

All (164) 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:27:LYS:NZ	1:C:40:CYS:SG	2.28	1.06
1:D:22:VAL:HG12	1:D:273[B]:CYS:SG	2.06	0.95
1:B:7:GLU:HG2	1:B:283:MET:HE1	1.49	0.94
1:C:22:VAL:HG12	1:C:273[B]:CYS:SG	2.10	0.91
1:A:243:TRP:CZ3	3:D:520:HOH:O	2.28	0.87
1:A:42[A]:ASN:HD21	1:A:46:LYS:H	1.22	0.83
1:B:42:ASN:HD22	1:B:42:ASN:C	1.91	0.78
1:C:13:GLN:HE21	1:C:13:GLN:HA	1.46	0.78
1:A:202:ILE:HD11	1:D:51:PRO:HD2	1.69	0.75
1:C:224:ASN:OD1	1:C:226:ARG:NH1	2.21	0.74
1:D:1:MET:C	1:D:1:MET:HE3	2.13	0.73
1:C:298:MET:CE	3:C:478:HOH:O	2.37	0.73
1:A:13:GLN:HG3	3:A:547:HOH:O	1.87	0.72
1:A:226:ARG:HH11	1:D:12:ASN:HD22	1.37	0.72
1:C:298:MET:HE3	3:C:478:HOH:O	1.89	0.72
1:D:292:THR:HG23	3:D:333:HOH:O	1.88	0.72
1:A:42[A]:ASN:ND2	1:A:44:ASP:OD2	2.24	0.70
1:B:270:HIS:HD2	3:B:392:HOH:O	1.75	0.70
1:D:84:THR:OG1	1:D:86:LYS:HD2	1.93	0.69
1:A:219[B]:LYS:NZ	3:A:597:HOH:O	2.23	0.68
1:B:22:VAL:HG23	1:B:273[A]:CYS:SG	2.33	0.68
1:B:263:GLN:O	1:B:264:ILE:HD12	1.94	0.68
1:D:85[B]:LYS:HE3	3:D:328:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:HIS:CE1	1:A:284:GLU:HB2	2.29	0.67
1:B:42:ASN:HB3	3:B:562:HOH:O	1.94	0.67
1:C:224:ASN:OD1	1:C:226:ARG:CZ	2.44	0.66
1:A:42[A]:ASN:ND2	1:A:46:LYS:H	1.93	0.65
1:C:11:THR:HG21	1:C:49:GLU:OE2	1.97	0.65
1:D:85[B]:LYS:CE	3:D:328:HOH:O	2.45	0.65
1:C:32:GLN:NE2	1:C:39:SER:OG	2.26	0.64
1:C:292:THR:HG23	3:C:398:HOH:O	1.98	0.64
1:D:33:HIS:HD2	3:D:368:HOH:O	1.81	0.64
1:B:7:GLU:OE1	1:B:264:ILE:CD1	2.47	0.63
1:B:4:LYS:HG2	1:B:292[A]:THR:OG1	1.98	0.62
1:C:273[B]:CYS:SG	1:C:274:PHE:N	2.73	0.61
1:D:1:MET:HE1	1:D:3:PHE:HD2	1.64	0.61
1:A:226:ARG:HH11	1:D:12:ASN:ND2	1.97	0.61
1:A:202:ILE:HD11	1:D:51:PRO:CD	2.31	0.61
1:B:226[B]:ARG:HH11	1:B:226[B]:ARG:HG3	1.66	0.60
1:A:237:ASP:OD1	1:A:252:THR:HG23	2.02	0.60
1:D:273[B]:CYS:SG	3:D:346:HOH:O	2.56	0.59
1:B:42:ASN:C	1:B:42:ASN:ND2	2.60	0.59
1:A:236:ILE:HD12	1:A:236:ILE:C	2.27	0.58
1:A:255:ASN:ND2	3:A:543:HOH:O	2.36	0.58
1:D:11:THR:OG1	1:D:49:GLU:OE2	2.21	0.58
1:B:270:HIS:HE1	1:B:284:GLU:OE1	1.87	0.57
1:A:270:HIS:HE1	1:A:284:GLU:HB2	1.69	0.56
1:B:265:LYS:HD3	3:B:551:HOH:O	2.04	0.56
1:B:162:ASN:ND2	1:B:183:SER:H	2.03	0.56
1:D:1:MET:HB2	1:D:295:LYS:O	2.06	0.56
1:D:84:THR:HG1	1:D:86:LYS:HD2	1.70	0.56
1:D:162:ASN:ND2	1:D:183:SER:H	2.04	0.56
1:B:78:ASN:HD21	1:B:99:SER:HB2	1.71	0.55
1:A:237:ASP:OD1	1:A:252:THR:CG2	2.54	0.55
1:D:291:LEU:C	1:D:291:LEU:HD23	2.31	0.55
1:A:1:MET:HB3	1:A:293:LEU:HB3	1.89	0.55
1:A:42[A]:ASN:HD21	1:A:46:LYS:N	2.00	0.54
1:B:7:GLU:OE1	1:B:264:ILE:HG12	2.08	0.54
1:A:243:TRP:HZ3	3:D:479:HOH:O	1.91	0.53
1:C:177:LYS:NZ	3:C:472:HOH:O	2.42	0.52
1:C:20:ILE:HD12	1:C:30:ILE:CD1	2.40	0.52
1:A:27:LYS:HD3	1:A:40[A]:CYS:SG	2.50	0.52
1:A:42[A]:ASN:ND2	1:A:46:LYS:N	2.58	0.52
1:B:120:ASN:ND2	1:B:141:SER:H	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:LYS:HA	1:D:265:LYS:CE	2.39	0.52
1:D:197:TRP:CD2	1:D:238:LEU:HD13	2.44	0.52
1:B:120:ASN:HD21	1:B:141:SER:H	1.58	0.52
1:B:78:ASN:ND2	1:B:99:SER:HB2	2.25	0.52
1:C:27:LYS:NZ	1:C:42:ASN:OD1	2.36	0.51
1:A:65:SER:OG	1:A:67:ASP:OD1	2.27	0.51
1:B:42:ASN:ND2	1:B:44:ASP:OD1	2.22	0.51
1:B:86:LYS:CG	3:B:588:HOH:O	2.58	0.51
1:C:20:ILE:HD12	1:C:30:ILE:HD12	1.94	0.50
1:B:85:LYS:HG2	3:B:382:HOH:O	2.12	0.50
1:A:13:GLN:CD	3:A:619:HOH:O	2.54	0.49
1:B:3:PHE:HA	1:B:293:LEU:HA	1.95	0.49
1:B:197:TRP:CD2	1:B:238:LEU:HD13	2.48	0.49
1:A:22[B]:VAL:HG22	1:A:28:VAL:HG22	1.94	0.49
1:D:85[A]:LYS:HG3	3:D:328:HOH:O	2.12	0.49
1:B:239:TRP:CD1	1:B:279:ILE:HD11	2.48	0.49
1:A:162:ASN:ND2	1:A:183:SER:H	2.11	0.48
1:D:1:MET:HE3	1:D:1:MET:O	2.13	0.48
1:B:265:LYS:NZ	3:B:554:HOH:O	2.46	0.48
1:B:78:ASN:ND2	1:B:99:SER:H	2.11	0.48
1:B:273[B]:CYS:SG	1:B:274:PHE:N	2.86	0.48
1:D:116:GLU:OE2	1:D:133:GLU:OE2	2.31	0.48
1:A:297:ASN:ND2	3:A:509:HOH:O	2.43	0.48
1:A:239:TRP:CD1	1:A:279:ILE:HD11	2.48	0.48
1:A:270:HIS:HD2	3:A:592:HOH:O	1.96	0.48
1:B:41:ILE:CD1	1:B:47:ILE:HG12	2.44	0.48
1:C:14:ASP:N	1:C:286:ASP:OD2	2.44	0.48
1:C:60:MET:HG3	1:C:75:ASN:HB2	1.95	0.48
1:D:102:TYR:HB2	1:D:117[A]:MET:HG3	1.95	0.48
1:C:11:THR:CG2	3:C:400:HOH:O	2.62	0.47
1:B:60:MET:HA	1:B:60:MET:HE2	1.97	0.47
1:D:12:ASN:C	3:D:500:HOH:O	2.58	0.47
1:A:118:ASN:HD22	1:A:118:ASN:N	2.12	0.46
1:B:6:GLN:HG2	1:B:290:LYS:HB2	1.97	0.46
1:D:60:MET:HA	1:D:60:MET:HE2	1.97	0.46
1:B:51:PRO:HB3	3:B:356:HOH:O	2.14	0.46
1:D:133:GLU:OE2	2:D:301:CL:CL	2.71	0.46
1:A:60:MET:SD	1:D:55:PRO:HG2	2.55	0.46
1:B:162:ASN:ND2	1:B:183:SER:OG	2.49	0.46
1:B:33:HIS:HD2	3:B:437:HOH:O	1.98	0.46
1:B:214[A]:GLU:OE1	3:B:557:HOH:O	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226[B]:ARG:HG3	1:B:226[B]:ARG:NH1	2.30	0.46
1:B:227:PRO:HA	1:B:241:THR:O	2.15	0.46
1:B:224:ASN:HB3	1:B:226[B]:ARG:HH21	1.80	0.46
1:B:22:VAL:HG22	1:B:28:VAL:HG22	1.98	0.46
1:B:42:ASN:HD21	1:B:44:ASP:CG	2.18	0.46
1:A:144[B]:SER:HB3	1:A:157:THR:OG1	2.16	0.46
1:A:4:LYS:HD2	1:A:5:LEU:N	2.31	0.45
1:B:7:GLU:OE1	1:B:264:ILE:HD13	2.15	0.45
1:C:224:ASN:OD1	1:C:226:ARG:NH2	2.50	0.45
1:D:167:ILE:HA	1:D:172:ASP:O	2.16	0.45
1:A:30[B]:ILE:HD13	1:A:288:ILE:HD11	1.99	0.45
1:C:227:PRO:HA	1:C:241:THR:O	2.17	0.45
1:D:84:THR:HG21	1:D:86:LYS:HZ2	1.81	0.45
1:B:224:ASN:HB3	1:B:226[B]:ARG:NH2	2.32	0.45
1:C:162:ASN:ND2	1:C:183:SER:H	2.15	0.45
1:C:270:HIS:HE1	1:C:284:GLU:HB2	1.81	0.45
1:A:143:PRO:HA	1:A:157:THR:O	2.18	0.44
1:D:84:THR:OG1	1:D:86:LYS:CD	2.64	0.44
1:A:298:MET:O	1:B:8:LEU:CD2	2.65	0.44
1:B:27:LYS:HD3	1:B:40[B]:CYS:SG	2.58	0.44
1:D:117[A]:MET:HE2	1:D:117[A]:MET:HB3	1.85	0.44
1:A:268:GLU:HB2	1:A:284:GLU:HB3	2.00	0.44
1:B:208:ARG:O	1:B:215:ILE:HA	2.18	0.44
1:A:291:LEU:HD23	1:A:292:THR:N	2.33	0.44
1:C:144[B]:SER:HB3	1:C:157:THR:OG1	2.18	0.44
1:D:117[B]:MET:HG2	1:D:142:TYR:HD2	1.82	0.44
1:B:166:ARG:O	1:B:173:ILE:HA	2.18	0.43
1:B:12:ASN:HB3	1:B:15:THR:HG21	2.00	0.43
1:A:208:ARG:O	1:A:215:ILE:HA	2.18	0.43
1:C:33:HIS:HD2	3:C:397:HOH:O	2.00	0.43
1:D:265:LYS:NZ	3:D:396:HOH:O	2.51	0.43
1:D:72:PHE:CZ	1:D:81:GLY:HA3	2.54	0.43
1:B:42:ASN:HB2	3:B:510:HOH:O	2.19	0.43
1:B:74:GLU:OE2	1:B:91:GLU:OE2	2.36	0.43
1:C:2:GLU:HB2	1:C:294:ILE:HB	2.00	0.43
1:B:7:GLU:OE1	1:B:264:ILE:CG1	2.67	0.43
1:C:143:PRO:HA	1:C:157:THR:O	2.19	0.43
1:A:60:MET:HG3	1:A:75:ASN:HB2	1.99	0.43
1:C:4:LYS:HB2	1:C:294:ILE:HD11	2.00	0.43
1:C:152:ASN:HD22	1:C:152:ASN:HA	1.66	0.42
1:C:72:PHE:CZ	1:C:81:GLY:HA3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:TRP:C	1:C:30:ILE:HD13	2.44	0.42
1:C:20:ILE:HG13	1:C:30:ILE:CD1	2.50	0.42
1:B:275:ASP:OD1	1:B:275:ASP:C	2.59	0.42
1:A:219[B]:LYS:CE	3:A:597:HOH:O	2.66	0.42
1:C:130:LYS:HE3	3:C:520:HOH:O	2.20	0.42
1:B:86:LYS:HG2	3:B:588:HOH:O	2.18	0.41
1:B:250:ARG:O	1:B:257:ILE:HA	2.20	0.41
1:D:126:THR:OG1	1:D:128:ASP:OD1	2.34	0.41
1:D:273[B]:CYS:SG	1:D:274:PHE:N	2.93	0.41
1:C:200:GLU:OE2	1:C:217:GLU:OE2	2.39	0.41
1:B:3:PHE:HB3	1:B:293:LEU:CD2	2.51	0.41
1:C:298:MET:HE2	1:C:298:MET:HB3	1.82	0.41
1:D:96:ASN:HB2	2:D:301:CL:CL	2.58	0.41
1:D:239:TRP:CD1	1:D:279:ILE:HD11	2.56	0.41
1:D:40[B]:CYS:SG	1:D:48:THR:HB	2.61	0.40
1:C:20:ILE:CD1	1:C:30:ILE:CD1	2.99	0.40
1:D:32:GLN:NE2	1:D:39:SER:OG	2.42	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	304/299 (102%)	288 (95%)	14 (5%)	2 (1%)	18	10
1	B	299/299 (100%)	287 (96%)	11 (4%)	1 (0%)	36	29
1	C	302/299 (101%)	288 (95%)	13 (4%)	1 (0%)	36	29
1	D	299/299 (100%)	286 (96%)	12 (4%)	1 (0%)	36	29
All	All	1204/1196 (101%)	1149 (95%)	50 (4%)	5 (0%)	30	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	ASP
1	B	186	VAL
1	A	186	VAL
1	D	186	VAL
1	C	186	VAL

5.3.2 Protein sidechains ⓘ

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	259/253 (102%)	251 (97%)	8 (3%)	35	29
1	B	255/253 (101%)	248 (97%)	7 (3%)	39	34
1	C	258/253 (102%)	243 (94%)	15 (6%)	18	10
1	D	255/253 (101%)	245 (96%)	10 (4%)	28	21
All	All	1027/1012 (102%)	987 (96%)	40 (4%)	28	21

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42[A]	ASN
1	A	42[C]	ASN
1	A	85	LYS
1	A	86	LYS
1	A	118	ASN
1	A	132	ARG
1	A	252	THR
1	A	265	LYS
1	B	2	GLU
1	B	7	GLU
1	B	42	ASN
1	B	86	LYS
1	B	128	ASP
1	B	253	SER
1	B	265	LYS
1	C	13	GLN
1	C	14	ASP

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Mol	Chain	Res	Type
1	C	25	LYS
1	C	46	LYS
1	C	47	ILE
1	C	67	ASP
1	C	124	ARG
1	C	127	ASP
1	C	139	LYS
1	C	254	ASN
1	C	277	GLU
1	C	292	THR
1	C	293	LEU
1	C	295	LYS
1	C	298	MET
1	D	1	MET
1	D	6	GLN
1	D	14	ASP
1	D	86	LYS
1	D	226	ARG
1	D	236	ILE
1	D	265	LYS
1	D	286	ASP
1	D	292	THR
1	D	295	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	32	GLN
1	A	118	ASN
1	A	162	ASN
1	A	270	HIS
1	A	297	ASN
1	B	6	GLN
1	B	12	ASN
1	B	32	GLN
1	B	33	HIS
1	B	42	ASN
1	B	78	ASN
1	B	120	ASN
1	B	159	ASN
1	B	160	GLN

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Mol	Chain	Res	Type
1	B	162	ASN
1	B	255	ASN
1	B	263	GLN
1	B	270	HIS
1	C	12	ASN
1	C	13	GLN
1	C	32	GLN
1	C	33	HIS
1	C	152	ASN
1	C	160	GLN
1	C	162	ASN
1	C	255	ASN
1	C	270	HIS
1	D	12	ASN
1	D	32	GLN
1	D	33	HIS
1	D	109	ASN
1	D	162	ASN
1	D	224	ASN
1	D	270	HIS

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 ⓘ

Of 5 ligands modelled in this entry, 5 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, 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	298/299 (99%)	0.04	12 (4%) 42 45	10, 20, 36, 47	14 (4%)
1	B	293/299 (97%)	-0.03	8 (2%) 56 60	12, 21, 35, 50	10 (3%)
1	C	299/299 (100%)	0.26	12 (4%) 42 45	12, 24, 37, 48	12 (4%)
1	D	295/299 (98%)	0.12	6 (2%) 65 69	12, 25, 36, 44	11 (3%)
All	All	1185/1196 (99%)	0.10	38 (3%) 50 54	10, 23, 37, 50	47 (3%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	5.6
1	C	299	GLU	4.1
1	B	3	PHE	3.8
1	A	2	GLU	3.6
1	A	298	MET	3.5
1	B	7	GLU	3.2
1	A	296	ASP	3.0
1	C	295	LYS	3.0
1	D	1	MET	3.0
1	B	16	GLY	2.9
1	A	15	THR	2.8
1	A	16	GLY	2.7
1	A	297	ASN	2.7
1	D	8	LEU	2.7
1	C	5	LEU	2.5
1	C	67	ASP	2.5
1	C	1	MET	2.5
1	C	13	GLN	2.5
1	A	243	TRP	2.5
1	D	3	PHE	2.4
1	C	16	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	295	LYS	2.3
1	B	294	ILE	2.3
1	C	3	PHE	2.3
1	C	8	LEU	2.3
1	C	296	ASP	2.2
1	B	15	THR	2.2
1	C	10	LEU	2.2
1	B	2	GLU	2.1
1	B	44	ASP	2.1
1	A	265	LYS	2.1
1	A	294	ILE	2.1
1	C	12	ASN	2.1
1	B	8	LEU	2.1
1	D	286	ASP	2.1
1	A	3	PHE	2.0
1	A	263	GLN	2.0
1	D	11	THR	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 ⓘ

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, 95th 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	CL	D	301	1/1	0.97	0.23	38,38,38,38	0
2	CL	D	300	1/1	0.98	0.15	25,25,25,25	0
2	CL	C	300	1/1	0.99	0.16	23,23,23,23	0
2	CL	A	300	1/1	0.99	0.13	20,20,20,20	0
2	CL	B	300	1/1	0.99	0.16	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.