



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:51 PM UTC

PDB ID : 9S4G / pdb_00009s4g
Title : Carbonic anhydrases from Candida parapsilosis
Authors : Dostal, J.
Deposited on : 2025-07-28
Resolution : 2.70 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

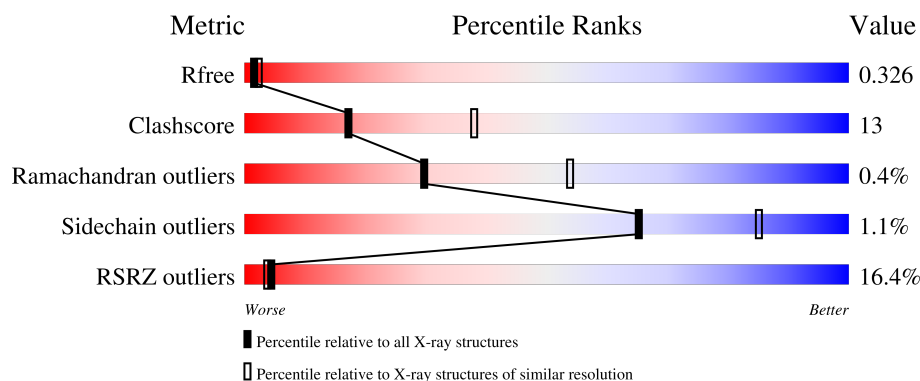
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	231	11% 67% 21% 12%
1	B	231	10% 73% 15% 12%
1	C	231	18% 73% 15% 12%
1	D	231	19% 68% 19% 12%

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
3	AZM	B	302	-	X	-	-
3	AZM	D	302	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11020 atoms, of which 5184 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 Carbonic anhydrase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	204	Total	C	H	N	O	S	0	0	0
			2806	926	1343	257	275	5			
1	B	204	Total	C	H	N	O	S	0	0	0
			2762	919	1307	250	281	5			
1	C	204	Total	C	H	N	O	S	0	0	0
			2645	888	1222	249	281	5			
1	D	203	Total	C	H	N	O	S	0	0	0
			2694	895	1266	255	273	5			

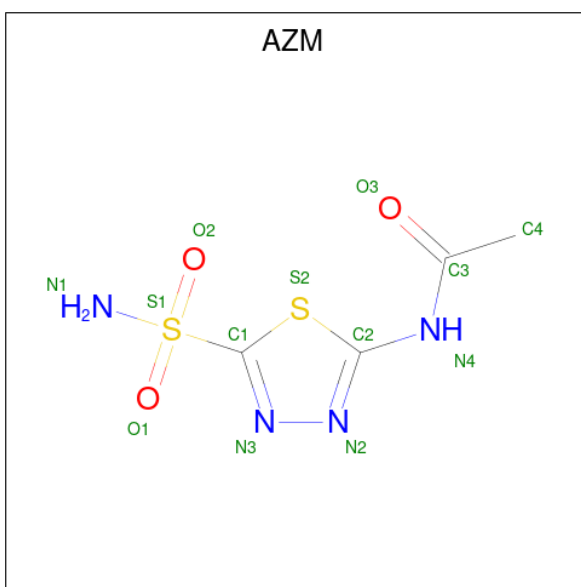
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	245	LEU	SER	conflict	UNP G8B6R8
B	245	LEU	SER	conflict	UNP G8B6R8
C	245	LEU	SER	conflict	UNP G8B6R8
D	245	LEU	SER	conflict	UNP G8B6R8

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is 5-ACETAMIDO-1,3,4-THIADIAZOLE-2-SULFONAMIDE (CCD ID: AZM) (formula: C₄H₆N₄O₃S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			19	4	6	4	3	2		
3	B	1	Total	C	H	N	O	S	0	0
			19	4	6	4	3	2		
3	C	1	Total	C	H	N	O	S	0	0
			19	4	6	4	3	2		
3	D	1	Total	C	H	N	O	S	0	0
			19	4	6	4	3	2		

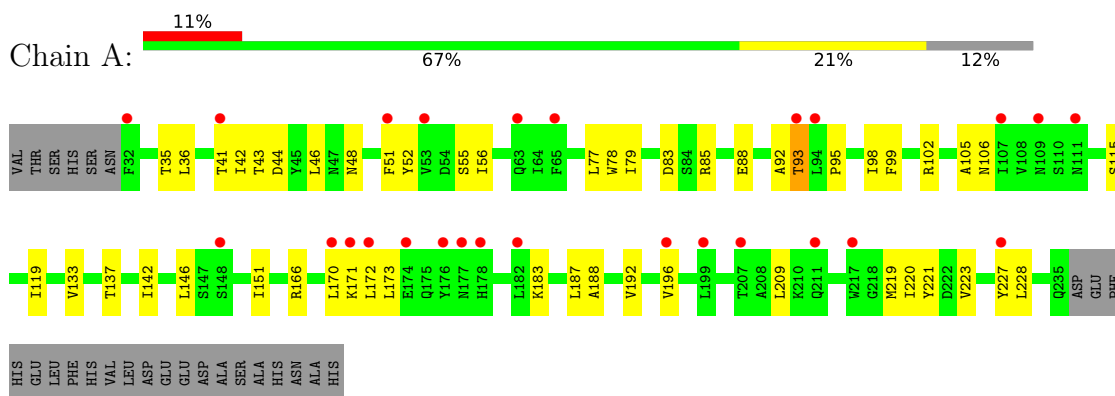
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	2	Total	H	O	0	0
			6	4	2		
4	B	2	Total	H	O	0	0
			6	4	2		
4	C	7	Total	H	O	0	0
			21	14	7		

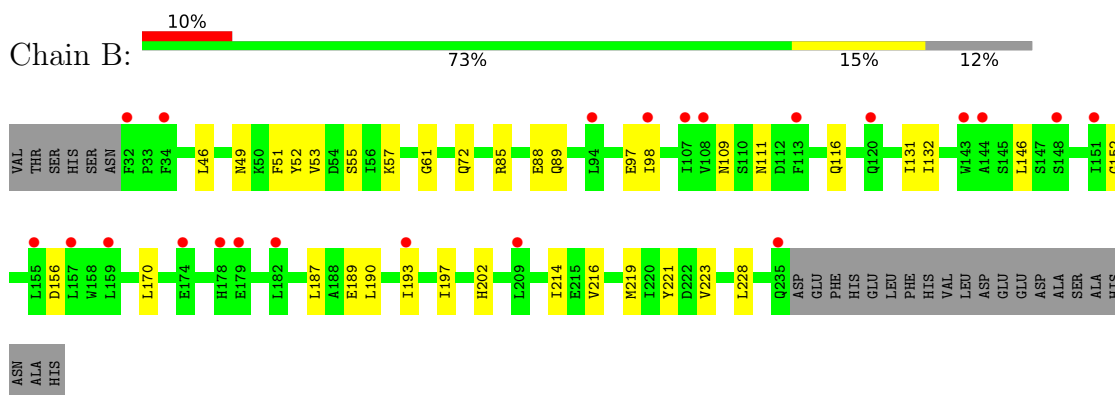
3 Residue-property plots

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.

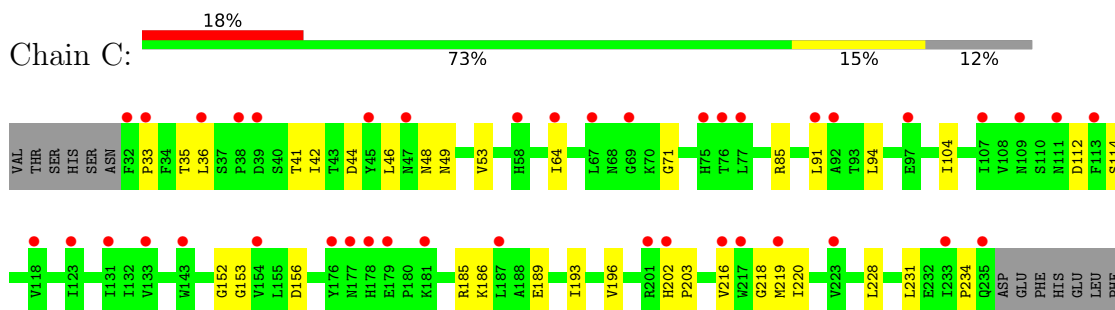
• Molecule 1: Carbonic anhydrase



• Molecule 1: Carbonic anhydrase

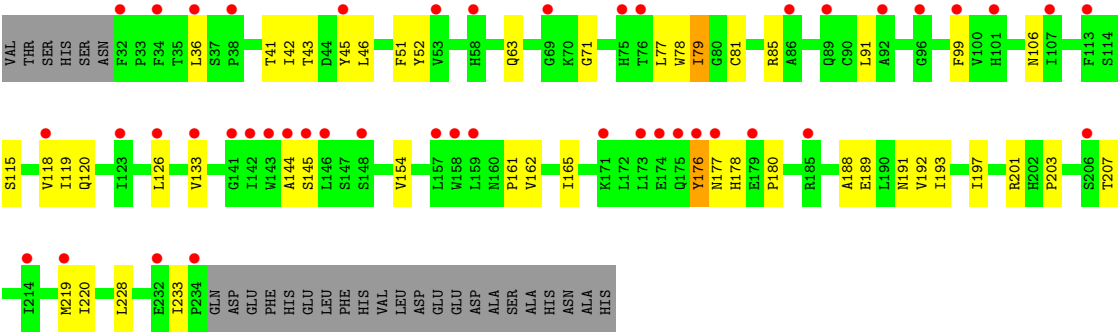


• Molecule 1: Carbonic anhydrase



HIS
VAL
LEU
ASP
GLU
GLU
ASP
ALA
SER
ALA
HIS
ASN
ALA
HIS

● Molecule 1: Carbonic anhydrase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.79Å 118.79Å 188.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.05 – 2.70 41.05 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.2 (41.05-2.70) 93.1 (41.05-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.272 , 0.329 0.271 , 0.326	Depositor DCC
R_{free} test set	2103 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	70.7	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11020	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.22	0/1493	0.31	0/2046
1	B	0.22	0/1486	0.32	0/2040
1	C	0.22	0/1453	0.31	0/1995
1	D	0.21	0/1457	0.31	0/1998
All	All	0.22	0/5889	0.31	0/8079

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1463	1343	1344	41	0
1	B	1455	1307	1308	30	0
1	C	1423	1222	1222	28	0
1	D	1428	1266	1272	46	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	13	6	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	6	6	0	0
3	C	13	6	6	1	0
3	D	13	6	6	2	0
4	A	2	4	0	0	0
4	B	2	4	0	1	0
4	C	7	14	0	0	0
All	All	5836	5184	5170	139	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 13.

All (139) 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:B:89:GLN:OE1	4:B:401:HOH:O	1.98	0.80
1:C:152:GLY:N	1:C:156:ASP:OD2	2.23	0.69
1:A:146:LEU:HD23	1:A:166:ARG:HD2	1.76	0.67
1:B:97:GLU:C	1:B:98:ILE:HD13	2.18	0.67
1:B:49:ASN:O	1:B:53:VAL:HG23	1.94	0.67
1:D:201:ARG:HG2	1:D:201:ARG:HH11	1.59	0.67
1:D:43:THR:HA	1:D:46:LEU:HD13	1.78	0.66
1:B:146:LEU:HD21	1:B:187:LEU:HD22	1.77	0.65
1:C:219:MET:C	1:C:220:ILE:HD13	2.21	0.65
1:D:192:VAL:HG21	1:D:220:ILE:HD11	1.81	0.62
1:B:85:ARG:HE	1:B:223:VAL:HG21	1.64	0.62
1:B:193:ILE:O	1:B:197:ILE:HD12	1.99	0.61
1:D:219:MET:O	1:D:220:ILE:HD13	2.01	0.60
1:D:91:LEU:HD11	1:D:228:LEU:HD11	1.81	0.60
1:A:35:THR:OG1	1:A:36:LEU:HD22	2.01	0.60
1:D:233:ILE:C	1:D:233:ILE:HD12	2.26	0.60
1:C:219:MET:O	1:C:220:ILE:HD13	2.02	0.59
1:D:203:PRO:O	1:D:207:THR:OG1	2.17	0.58
1:C:189:GLU:HB3	1:C:231:LEU:HD21	1.86	0.58
1:A:83:ASP:OD2	1:B:72:GLN:NE2	2.37	0.57
1:B:197:ILE:HD12	1:B:197:ILE:H	1.68	0.57
1:D:189:GLU:O	1:D:193:ILE:HD12	2.04	0.57
1:D:176:TYR:O	1:D:178:HIS:N	2.36	0.57
1:A:151:ILE:HD12	1:A:151:ILE:N	2.21	0.56
1:D:119:ILE:HD12	1:D:119:ILE:N	2.20	0.56
1:D:201:ARG:HG2	1:D:201:ARG:NH1	2.20	0.56
1:A:83:ASP:O	1:A:102:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:LEU:CD1	1:D:228:LEU:HD11	2.36	0.55
1:B:109:ASN:OD1	1:B:111:ASN:N	2.30	0.55
1:D:188:ALA:O	1:D:192:VAL:HG23	2.07	0.55
1:D:145:SER:HB3	1:D:162:VAL:HG12	1.88	0.55
1:D:46:LEU:H	1:D:46:LEU:HD12	1.72	0.54
1:D:91:LEU:HD11	1:D:228:LEU:CD1	2.37	0.54
1:A:78:TRP:N	1:A:99:PHE:O	2.39	0.54
1:A:115:SER:O	1:A:119:ILE:HD12	2.06	0.54
1:B:97:GLU:O	1:B:98:ILE:HD13	2.06	0.54
1:D:42:ILE:O	1:D:46:LEU:HD12	2.08	0.53
1:B:131:ILE:HD11	1:B:214:ILE:HD11	1.89	0.53
1:C:189:GLU:OE1	1:C:189:GLU:N	2.43	0.52
1:C:85:ARG:NH1	1:D:71:GLY:O	2.38	0.52
1:D:119:ILE:HD12	1:D:119:ILE:H	1.74	0.52
1:A:133:VAL:HG11	1:A:196:VAL:HG22	1.91	0.52
1:D:162:VAL:HG22	1:D:191:ASN:ND2	2.25	0.52
1:A:51:PHE:C	1:A:51:PHE:CD1	2.88	0.52
1:B:51:PHE:CD1	1:B:51:PHE:C	2.85	0.52
1:C:91:LEU:CD2	1:C:228:LEU:HD11	2.42	0.50
1:C:42:ILE:O	1:C:46:LEU:HD12	2.12	0.50
1:D:42:ILE:HG13	1:D:46:LEU:HD11	1.94	0.50
1:A:56:ILE:HD12	1:A:56:ILE:N	2.27	0.49
1:B:152:GLY:N	1:B:156:ASP:OD2	2.28	0.49
1:A:227:TYR:CE1	1:B:53:VAL:HG11	2.47	0.49
1:D:144:ALA:HB2	3:D:302:AZM:H41	1.94	0.49
1:D:77:LEU:HD23	1:D:78:TRP:N	2.28	0.49
1:C:185:ARG:O	1:C:189:GLU:OE1	2.31	0.49
1:C:49:ASN:O	1:C:53:VAL:HG23	2.13	0.48
1:D:162:VAL:CG2	1:D:191:ASN:ND2	2.76	0.48
1:A:142:ILE:HD12	1:A:188:ALA:HA	1.95	0.48
1:A:88:GLU:OE1	1:A:88:GLU:N	2.46	0.48
1:D:161:PRO:O	1:D:165:ILE:HG13	2.14	0.48
1:C:64:ILE:HD12	1:C:94:LEU:HD13	1.96	0.47
1:A:170:LEU:C	1:A:170:LEU:HD23	2.39	0.47
1:A:192:VAL:O	1:A:196:VAL:HG23	2.14	0.47
1:D:42:ILE:HG23	1:D:43:THR:H	1.79	0.47
1:A:35:THR:OG1	1:A:36:LEU:CD2	2.62	0.47
1:B:109:ASN:OD1	1:B:109:ASN:C	2.57	0.47
1:B:131:ILE:CD1	1:B:214:ILE:HD11	2.45	0.47
1:A:219:MET:O	1:A:220:ILE:HD13	2.15	0.47
1:D:42:ILE:O	1:D:45:TYR:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:O	1:A:52:TYR:C	2.58	0.46
1:A:52:TYR:O	1:A:56:ILE:CD1	2.63	0.46
1:A:188:ALA:O	1:A:192:VAL:HG23	2.15	0.46
1:C:112:ASP:OD1	1:C:114:SER:N	2.45	0.46
1:C:189:GLU:H	1:C:189:GLU:CD	2.22	0.46
1:D:177:ASN:C	1:D:180:PRO:HD3	2.40	0.46
1:A:172:LEU:HD23	1:A:172:LEU:C	2.40	0.46
1:D:197:ILE:O	1:D:201:ARG:HG3	2.16	0.46
1:D:233:ILE:HD12	1:D:233:ILE:O	2.16	0.46
1:A:41:THR:O	1:A:44:ASP:HB2	2.16	0.46
1:D:145:SER:CB	1:D:162:VAL:HG11	2.45	0.46
1:B:57:LYS:O	1:B:61:GLY:N	2.46	0.46
1:C:104:ILE:HG23	3:C:302:AZM:N3	2.31	0.46
1:B:85:ARG:NE	1:B:223:VAL:HG21	2.31	0.46
1:B:132:ILE:HD13	1:B:219:MET:CE	2.46	0.45
1:B:116:GLN:OE1	1:B:202:HIS:CD2	2.70	0.45
1:D:145:SER:CB	1:D:162:VAL:CG1	2.94	0.45
1:A:146:LEU:HD13	1:A:183:LYS:HD2	1.98	0.45
1:D:77:LEU:HD23	1:D:77:LEU:C	2.42	0.44
1:A:41:THR:CG2	1:A:42:ILE:N	2.80	0.44
1:A:41:THR:HG22	1:A:42:ILE:N	2.33	0.44
1:D:46:LEU:HD12	1:D:46:LEU:N	2.32	0.44
1:A:79:ILE:O	1:A:133:VAL:HA	2.18	0.44
1:A:95:PRO:HD3	1:B:89:GLN:NE2	2.31	0.44
1:C:153:GLY:HA3	1:D:120:GLN:HE22	1.82	0.44
1:C:202:HIS:ND1	1:C:203:PRO:HD2	2.32	0.44
1:B:51:PHE:CE1	1:B:55:SER:OG	2.71	0.44
3:A:302:AZM:O3	3:A:302:AZM:S2	2.75	0.44
1:B:51:PHE:O	1:B:52:TYR:C	2.61	0.44
1:A:137:THR:OG1	1:A:223:VAL:HG12	2.18	0.43
1:A:146:LEU:HD21	1:A:187:LEU:HD22	1.99	0.43
1:A:170:LEU:O	1:A:171:LYS:C	2.61	0.43
1:B:170:LEU:HD12	1:B:170:LEU:O	2.18	0.43
1:A:41:THR:HG22	1:A:43:THR:H	1.83	0.43
1:D:99:PHE:CE1	1:D:126:LEU:HD12	2.53	0.43
1:D:42:ILE:HG23	1:D:43:THR:N	2.34	0.43
1:B:189:GLU:O	1:B:193:ILE:HG13	2.18	0.43
1:A:119:ILE:HD12	1:A:119:ILE:H	1.82	0.43
1:C:91:LEU:HD21	1:C:228:LEU:HD11	2.01	0.43
1:C:218:GLY:O	1:C:231:LEU:N	2.51	0.43
1:C:193:ILE:HD13	1:C:234:PRO:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:THR:HG22	1:D:42:ILE:N	2.33	0.43
1:A:77:LEU:HA	1:A:99:PHE:O	2.19	0.42
1:A:85:ARG:HD2	1:A:223:VAL:CG2	2.48	0.42
1:D:154:VAL:O	1:D:154:VAL:HG12	2.20	0.42
1:D:79:ILE:O	1:D:133:VAL:HA	2.19	0.42
1:C:186:LYS:C	1:C:189:GLU:OE1	2.63	0.42
1:B:146:LEU:HD21	1:B:187:LEU:CD2	2.47	0.42
1:B:190:LEU:HA	1:B:193:ILE:HD12	2.01	0.41
1:D:81:CYS:SG	3:D:302:AZM:O1	2.78	0.41
1:A:172:LEU:HD23	1:A:173:LEU:N	2.35	0.41
1:B:131:ILE:HD12	1:B:216:VAL:HG12	2.02	0.41
1:B:221:TYR:HA	1:B:228:LEU:HD23	2.03	0.41
1:C:48:ASN:OD1	1:C:48:ASN:N	2.51	0.41
1:A:44:ASP:O	1:A:48:ASN:OD1	2.38	0.41
1:A:93:THR:HG21	1:A:98:ILE:HD12	2.02	0.41
1:C:33:PRO:HG3	1:D:63:GLN:NE2	2.36	0.41
1:C:35:THR:OG1	1:C:36:LEU:HD22	2.21	0.41
1:A:51:PHE:CE1	1:A:55:SER:HB2	2.56	0.41
1:A:221:TYR:HA	1:A:228:LEU:HD23	2.03	0.41
1:B:46:LEU:H	1:B:46:LEU:HD22	1.85	0.41
1:C:186:LYS:O	1:C:189:GLU:OE1	2.39	0.40
1:D:51:PHE:O	1:D:52:TYR:C	2.64	0.40
1:D:99:PHE:CD1	1:D:126:LEU:HD12	2.56	0.40
1:C:41:THR:CG2	1:C:42:ILE:N	2.84	0.40
1:D:115:SER:O	1:D:118:VAL:N	2.53	0.40
1:C:44:ASP:O	1:C:48:ASN:OD1	2.40	0.40
1:C:71:GLY:C	1:D:85:ARG:HH12	2.29	0.40
1:A:151:ILE:HD12	1:A:151:ILE:H	1.87	0.40
1:A:105:ALA:O	1:A:106:ASN:C	2.65	0.40
1:C:196:VAL:HG23	1:C:216:VAL:HG11	2.04	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	202/231 (87%)	189 (94%)	12 (6%)	1 (0%)	24	48
1	B	202/231 (87%)	186 (92%)	16 (8%)	0	100	100
1	C	202/231 (87%)	190 (94%)	12 (6%)	0	100	100
1	D	201/231 (87%)	186 (92%)	13 (6%)	2 (1%)	12	32
All	All	807/924 (87%)	751 (93%)	53 (7%)	3 (0%)	30	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ALA
1	D	106	ASN
1	D	176	TYR

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	142/200 (71%)	139 (98%)	3 (2%)	47	75
1	B	142/200 (71%)	141 (99%)	1 (1%)	76	90
1	C	132/200 (66%)	132 (100%)	0	100	100
1	D	135/200 (68%)	133 (98%)	2 (2%)	57	81
All	All	551/800 (69%)	545 (99%)	6 (1%)	65	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	93	THR
1	A	209	LEU
1	B	88	GLU
1	D	36	LEU

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Mol	Chain	Res	Type
1	D	79	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	169	ASN
1	B	175	GLN
1	C	72	GLN
1	C	116	GLN
1	D	120	GLN
1	D	191	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	AZM	C	302	2	13,13,13	3.88	6 (46%)	19,19,19	3.53	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AZM	B	302	2	13,13,13	3.74	6 (46%)	19,19,19	3.86	6 (31%)
3	AZM	D	302	2	13,13,13	4.06	8 (61%)	19,19,19	3.36	5 (26%)
3	AZM	A	302	2	13,13,13	4.07	7 (53%)	19,19,19	3.51	4 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AZM	C	302	2	-	4/10/10/10	0/1/1/1
3	AZM	B	302	2	-	10/10/10/10	0/1/1/1
3	AZM	D	302	2	-	6/10/10/10	0/1/1/1
3	AZM	A	302	2	-	4/10/10/10	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	AZM	C1-S1	-9.14	1.71	1.78
3	D	302	AZM	C1-S1	-8.71	1.71	1.78
3	A	302	AZM	C1-S1	-8.61	1.71	1.78
3	A	302	AZM	C2-S2	-7.84	1.60	1.73
3	B	302	AZM	C1-S1	-7.80	1.72	1.78
3	D	302	AZM	C2-S2	-7.76	1.60	1.73
3	C	302	AZM	C2-S2	-7.58	1.61	1.73
3	B	302	AZM	C2-S2	-7.48	1.61	1.73
3	D	302	AZM	C1-N3	6.32	1.34	1.29
3	A	302	AZM	C1-N3	6.10	1.34	1.29
3	B	302	AZM	C1-N3	5.19	1.33	1.29
3	C	302	AZM	C1-N3	4.27	1.32	1.29
3	A	302	AZM	C2-N2	3.83	1.36	1.31
3	D	302	AZM	C2-N2	3.54	1.36	1.31
3	C	302	AZM	C2-N2	3.50	1.36	1.31
3	B	302	AZM	C2-N2	3.44	1.36	1.31
3	A	302	AZM	N3-N2	2.93	1.45	1.39
3	D	302	AZM	N3-N2	2.78	1.45	1.39
3	B	302	AZM	N3-N2	2.59	1.45	1.39
3	C	302	AZM	N3-N2	2.58	1.45	1.39
3	B	302	AZM	C1-S2	-2.56	1.70	1.73
3	C	302	AZM	O2-S1	2.53	1.47	1.43
3	A	302	AZM	O2-S1	2.51	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	AZM	C1-S2	-2.06	1.70	1.73
3	D	302	AZM	O2-S1	2.06	1.46	1.43
3	D	302	AZM	C3-N4	-2.03	1.32	1.37
3	D	302	AZM	O1-S1	2.03	1.46	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	AZM	C1-S2-C2	11.61	90.98	85.47
3	D	302	AZM	C1-N3-N2	-10.45	105.00	111.48
3	A	302	AZM	C1-S2-C2	10.34	90.38	85.47
3	C	302	AZM	C1-S2-C2	9.98	90.21	85.47
3	A	302	AZM	C1-N3-N2	-9.84	105.38	111.48
3	B	302	AZM	C1-N3-N2	-9.50	105.59	111.48
3	C	302	AZM	C1-N3-N2	-9.02	105.89	111.48
3	D	302	AZM	C1-S2-C2	8.23	89.38	85.47
3	B	302	AZM	O2-S1-O1	-3.93	114.64	120.27
3	A	302	AZM	O2-S1-O1	-3.71	114.96	120.27
3	C	302	AZM	O2-S1-O1	-3.67	115.03	120.27
3	B	302	AZM	N4-C2-N2	-3.56	117.63	120.81
3	C	302	AZM	N4-C2-N2	-3.56	117.64	120.81
3	C	302	AZM	S2-C2-N4	-3.27	119.33	123.72
3	B	302	AZM	S2-C2-N4	-3.26	119.36	123.72
3	D	302	AZM	O2-S1-O1	-3.17	115.75	120.27
3	C	302	AZM	C3-N4-C2	-2.85	119.35	124.05
3	D	302	AZM	C3-N4-C2	-2.83	119.39	124.05
3	D	302	AZM	S2-C1-N3	2.66	117.50	116.10
3	A	302	AZM	O1-S1-C1	2.10	108.77	105.65
3	B	302	AZM	C3-N4-C2	-2.07	120.64	124.05

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	AZM	C4-C3-N4-C2
3	A	302	AZM	O3-C3-N4-C2
3	B	302	AZM	N2-C2-N4-C3
3	B	302	AZM	S2-C2-N4-C3
3	B	302	AZM	C4-C3-N4-C2
3	B	302	AZM	O3-C3-N4-C2
3	C	302	AZM	N2-C2-N4-C3
3	C	302	AZM	S2-C2-N4-C3

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Mol	Chain	Res	Type	Atoms
3	C	302	AZM	C4-C3-N4-C2
3	C	302	AZM	O3-C3-N4-C2
3	D	302	AZM	N2-C2-N4-C3
3	D	302	AZM	S2-C2-N4-C3
3	D	302	AZM	C4-C3-N4-C2
3	D	302	AZM	O3-C3-N4-C2
3	A	302	AZM	S2-C1-S1-O2
3	B	302	AZM	N3-C1-S1-N1
3	B	302	AZM	N3-C1-S1-O2
3	B	302	AZM	S2-C1-S1-N1
3	A	302	AZM	N3-C1-S1-O2
3	B	302	AZM	S2-C1-S1-O1
3	B	302	AZM	S2-C1-S1-O2
3	D	302	AZM	S2-C1-S1-O2
3	B	302	AZM	N3-C1-S1-O1
3	D	302	AZM	N3-C1-S1-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302	AZM	1	0
3	D	302	AZM	2	0
3	A	302	AZM	1	0

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	204/231 (88%)	0.94	26 (12%) 8 7	63, 89, 125, 148	0
1	B	204/231 (88%)	1.00	22 (10%) 11 9	67, 92, 131, 165	0
1	C	204/231 (88%)	1.19	41 (20%) 3 2	73, 99, 143, 176	0
1	D	203/231 (87%)	1.21	45 (22%) 2 2	72, 99, 144, 187	0
All	All	815/924 (88%)	1.09	134 (16%) 4 4	63, 95, 140, 187	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235	GLN	5.9
1	D	32	PHE	5.7
1	B	157	LEU	5.4
1	C	176	TYR	5.3
1	C	92	ALA	5.0
1	B	94	LEU	4.9
1	D	92	ALA	4.7
1	C	178	HIS	4.6
1	D	45	TYR	4.4
1	C	113	PHE	4.2
1	B	148	SER	4.1
1	C	32	PHE	4.0
1	C	179	GLU	4.0
1	C	75	HIS	3.9
1	B	32	PHE	3.9
1	D	113	PHE	3.9
1	D	146	LEU	3.9
1	C	154	VAL	3.7
1	B	98	ILE	3.7
1	D	144	ALA	3.7
1	B	182	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	144	ALA	3.6
1	D	176	TYR	3.5
1	B	178	HIS	3.5
1	D	177	ASN	3.4
1	D	148	SER	3.4
1	D	173	LEU	3.4
1	B	143	TRP	3.4
1	D	175	GLN	3.4
1	C	111	ASN	3.4
1	B	113	PHE	3.3
1	B	34	PHE	3.3
1	C	123	ILE	3.3
1	D	36	LEU	3.3
1	B	174	GLU	3.2
1	A	174	GLU	3.2
1	B	193	ILE	3.2
1	D	89	GLN	3.1
1	A	111	ASN	3.1
1	B	159	LEU	3.1
1	D	69	GLY	3.0
1	C	133	VAL	3.0
1	C	177	ASN	3.0
1	D	142	ILE	3.0
1	A	63	GLN	3.0
1	D	123	ILE	3.0
1	C	118	VAL	2.9
1	D	206	SER	2.9
1	A	177	ASN	2.9
1	B	108	VAL	2.9
1	C	187	LEU	2.9
1	C	216	VAL	2.9
1	A	41	THR	2.8
1	C	38	PRO	2.8
1	D	118	VAL	2.8
1	A	178	HIS	2.7
1	D	34	PHE	2.7
1	D	214	ILE	2.7
1	A	109	ASN	2.7
1	C	109	ASN	2.7
1	B	209	LEU	2.7
1	D	96	GLY	2.7
1	C	47	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	145	SER	2.7
1	C	107	ILE	2.7
1	D	107	ILE	2.7
1	D	58	HIS	2.7
1	A	211	GLN	2.6
1	C	45	TYR	2.6
1	D	76	THR	2.6
1	B	107	ILE	2.6
1	A	51	PHE	2.5
1	D	157	LEU	2.5
1	C	69	GLY	2.5
1	A	207	THR	2.5
1	A	182	LEU	2.5
1	D	234	PRO	2.5
1	C	64	ILE	2.5
1	C	235	GLN	2.5
1	A	217	TRP	2.4
1	D	143	TRP	2.4
1	C	217	TRP	2.4
1	A	170	LEU	2.4
1	B	155	LEU	2.4
1	C	76	THR	2.4
1	D	232	GLU	2.4
1	D	219	MET	2.4
1	C	219	MET	2.4
1	C	233	ILE	2.3
1	A	32	PHE	2.3
1	D	99	PHE	2.3
1	A	199	LEU	2.3
1	C	91	LEU	2.3
1	C	131	ILE	2.3
1	C	202	HIS	2.3
1	B	179	GLU	2.3
1	D	174	GLU	2.3
1	C	223	VAL	2.3
1	C	67	LEU	2.3
1	C	181	LYS	2.3
1	D	38	PRO	2.3
1	D	101	HIS	2.2
1	A	171	LYS	2.2
1	A	93	THR	2.2
1	C	143	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	53	VAL	2.2
1	A	107	ILE	2.2
1	D	86	ALA	2.2
1	D	126	LEU	2.2
1	C	77	LEU	2.2
1	D	133	VAL	2.2
1	A	94	LEU	2.2
1	D	159	LEU	2.2
1	D	53	VAL	2.2
1	C	97	GLU	2.1
1	A	172	LEU	2.1
1	C	36	LEU	2.1
1	D	179	GLU	2.1
1	D	75	HIS	2.1
1	D	171	LYS	2.1
1	B	120	GLN	2.1
1	C	58	HIS	2.1
1	A	65	PHE	2.1
1	B	151	ILE	2.1
1	A	196	VAL	2.1
1	C	201	ARG	2.0
1	D	185	ARG	2.0
1	D	141	GLY	2.0
1	A	176	TYR	2.0
1	A	227	TYR	2.0
1	C	39	ASP	2.0
1	A	148	SER	2.0
1	D	158	TRP	2.0
1	C	33	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	AZM	B	302	13/13	0.93	0.11	69,84,123,123	0
3	AZM	C	302	13/13	0.94	0.13	82,90,184,184	0
3	AZM	A	302	13/13	0.96	0.09	75,79,93,93	0
3	AZM	D	302	13/13	0.96	0.09	81,94,113,118	0
2	ZN	C	301	1/1	0.99	0.07	78,78,78,78	0
2	ZN	D	301	1/1	0.99	0.03	75,75,75,75	0
2	ZN	A	301	1/1	1.00	0.04	66,66,66,66	0
2	ZN	B	301	1/1	1.00	0.02	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.