



Full wwPDB EM Validation Report ⓘ

May 24, 2026 – 02:07 AM JST

PDB ID : 9W3W / pdb_00009w3w
EMDB ID : EMD-65611
Title : Structure of Csm6 from *Actinomyces procaprae* in complex with cyclic penta-adenylate
Authors : Lin, Z.; Gao, H.; Shi, R.; Yang, M.; Liu, Y.
Deposited on : 2025-07-30
Resolution : 2.67 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

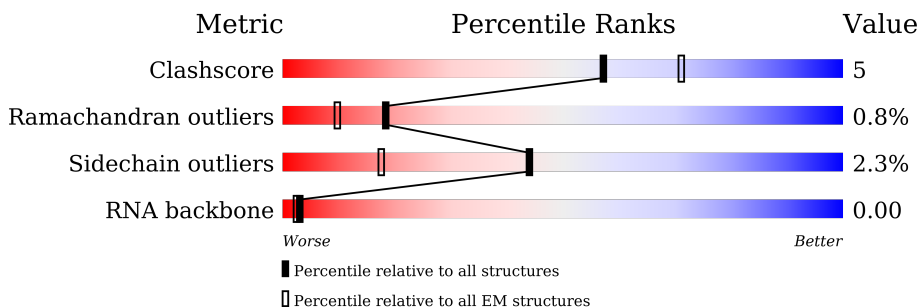
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.67 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	5	20% 60% 20%
1	2	5	20% 60% 20%
1	3	5	20% 60% 20%
1	4	5	60% 40%
2	A	797	86% 10% ..
2	B	797	87% 9% ..
2	C	797	87% 11% ..
2	D	797	87% 9% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24048 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 RNA chain called RNA (5'-R(P*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	5	Total 110	C 50	N 25	O 30	P 5	0	0
1	2	5	Total 110	C 50	N 25	O 30	P 5	0	0
1	3	5	Total 110	C 50	N 25	O 30	P 5	0	0
1	4	5	Total 110	C 50	N 25	O 30	P 5	0	0

- Molecule 2 is a protein called Csm6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	783	Total 5902	C 3662	N 1077	O 1139	S 24	0	0
2	B	783	Total 5902	C 3662	N 1077	O 1139	S 24	0	0
2	C	783	Total 5902	C 3662	N 1077	O 1139	S 24	0	0
2	D	783	Total 5902	C 3662	N 1077	O 1139	S 24	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. 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. 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: RNA (5'-R(P*AP*AP*AP*AP*A)-3')



- Molecule 1: RNA (5'-R(P*AP*AP*AP*AP*A)-3')



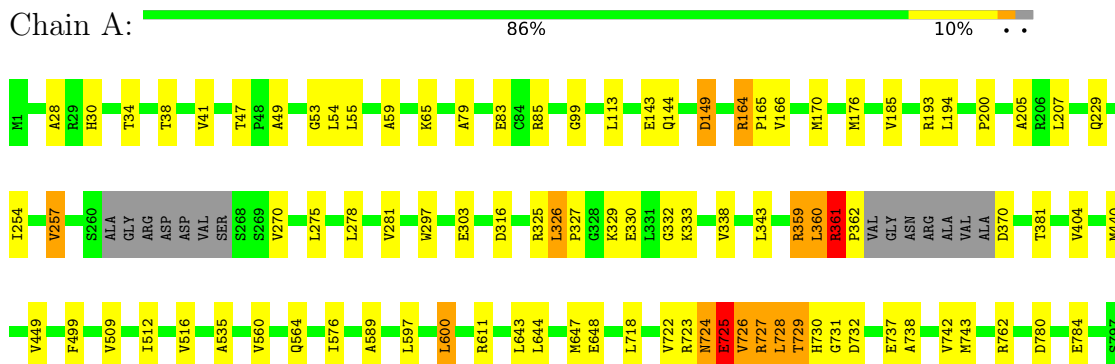
- Molecule 1: RNA (5'-R(P*AP*AP*AP*AP*A)-3')



- Molecule 1: RNA (5'-R(P*AP*AP*AP*AP*A)-3')



- Molecule 2: Csm6



- Molecule 2: Csm6

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143783	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS TITAN THEMIS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor

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	1	0.50	0/124	1.01	0/191
1	2	0.43	0/124	0.87	0/191
1	3	0.42	0/124	0.91	0/191
1	4	0.46	0/124	0.99	0/191
2	A	0.22	1/5997 (0.0%)	0.40	0/8118
2	B	0.19	1/5997 (0.0%)	0.39	0/8118
2	C	0.18	0/5997	0.40	2/8118 (0.0%)
2	D	0.17	0/5997	0.38	0/8118
All	All	0.20	2/24484 (0.0%)	0.41	2/33236 (0.0%)

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	1
2	B	0	1
2	C	0	1
2	D	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	360	LEU	CA-C	-5.11	1.46	1.52
2	A	360	LEU	CA-C	-5.08	1.46	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	360	LEU	N-CA-C	-6.92	103.31	112.72
2	C	726	VAL	N-CA-C	5.31	116.55	108.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	316	ASP	Peptide
2	B	316	ASP	Peptide
2	C	316	ASP	Peptide
2	D	316	ASP	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	1	110	0	55	1	0
1	2	110	0	55	1	0
1	3	110	0	55	1	0
1	4	110	0	56	6	0
2	A	5902	0	5828	59	0
2	B	5902	0	5828	53	0
2	C	5902	0	5828	58	0
2	D	5902	0	5828	56	0
All	All	24048	0	23533	227	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (227) 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:C:361:ARG:HB3	2:C:362:PRO:HD3	1.56	0.88
2:C:727:ARG:HH11	2:C:735:VAL:HG23	1.40	0.87
2:A:361:ARG:HD2	2:A:362:PRO:HD2	1.57	0.86
2:C:79:ALA:HB2	2:C:205:ALA:H	1.44	0.82
2:A:79:ALA:HB2	2:A:205:ALA:H	1.44	0.82
2:D:79:ALA:HB2	2:D:205:ALA:H	1.44	0.82
2:B:79:ALA:HB2	2:B:205:ALA:H	1.44	0.82
2:D:727:ARG:HE	2:D:734:SER:HA	1.45	0.82
2:B:55:LEU:HD13	2:B:113:LEU:HD23	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:LEU:HD13	2:D:113:LEU:HD23	1.69	0.75
2:A:359:ARG:C	2:A:361:ARG:H	1.94	0.75
2:A:55:LEU:HD13	2:A:113:LEU:HD23	1.69	0.74
2:C:55:LEU:HD13	2:C:113:LEU:HD23	1.69	0.74
2:C:660:ASP:HB2	2:C:727:ARG:HH12	1.52	0.73
2:A:718:LEU:HD13	2:A:743:MET:HE1	1.72	0.72
2:C:718:LEU:HD13	2:C:743:MET:HE1	1.72	0.72
2:D:718:LEU:HD13	2:D:743:MET:HE1	1.72	0.71
2:B:718:LEU:HD13	2:B:743:MET:HE1	1.72	0.71
2:C:292:LEU:CD2	2:C:295:ARG:NH2	2.56	0.69
2:B:359:ARG:C	2:B:361:ARG:H	2.02	0.67
2:D:360:LEU:O	2:D:361:ARG:C	2.38	0.65
2:D:254:ILE:HD11	2:D:281:VAL:HG21	1.80	0.63
2:B:254:ILE:HD11	2:B:281:VAL:HG21	1.80	0.63
2:B:361:ARG:O	2:B:362:PRO:C	2.41	0.63
2:D:143:GLU:HG3	2:D:144:GLN:H	1.64	0.63
2:A:193:ARG:HH21	2:A:207:LEU:HD23	1.64	0.63
2:B:143:GLU:HG3	2:B:144:GLN:H	1.64	0.63
2:C:193:ARG:HH21	2:C:207:LEU:HD23	1.64	0.63
2:D:727:ARG:NE	2:D:734:SER:HA	2.14	0.63
2:A:359:ARG:C	2:A:361:ARG:N	2.53	0.62
2:A:143:GLU:HG3	2:A:144:GLN:H	1.64	0.62
2:C:143:GLU:HG3	2:C:144:GLN:H	1.64	0.62
2:D:193:ARG:HH21	2:D:207:LEU:HD23	1.64	0.62
2:A:254:ILE:HD11	2:A:281:VAL:HG21	1.80	0.62
2:B:193:ARG:HH21	2:B:207:LEU:HD23	1.64	0.62
2:C:254:ILE:HD11	2:C:281:VAL:HG21	1.80	0.62
2:B:440:MET:HE3	2:B:600:LEU:HG	1.82	0.61
2:D:440:MET:HE3	2:D:600:LEU:HG	1.82	0.61
2:A:65:LYS:HE2	2:A:65:LYS:HA	1.82	0.61
2:C:65:LYS:HE2	2:C:65:LYS:HA	1.82	0.61
2:D:65:LYS:HA	2:D:65:LYS:HE2	1.82	0.61
2:C:667:VAL:HG12	2:C:723:ARG:HD3	1.83	0.61
2:B:65:LYS:HA	2:B:65:LYS:HE2	1.82	0.61
1:4:3:A:H8	2:D:411:GLY:HA2	1.65	0.61
2:C:440:MET:HE3	2:C:600:LEU:HG	1.82	0.61
2:A:440:MET:HE3	2:A:600:LEU:HG	1.82	0.61
2:A:724:ASN:O	2:A:725:GLU:HB2	2.01	0.60
2:B:360:LEU:O	2:B:361:ARG:C	2.43	0.60
1:4:5:A:H2	2:D:100:ASP:H	1.49	0.59
2:B:359:ARG:C	2:B:361:ARG:N	2.60	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:360:LEU:O	2:A:361:ARG:C	2.45	0.59
2:B:718:LEU:O	2:B:722:VAL:HG23	2.03	0.58
2:C:361:ARG:HB3	2:C:362:PRO:CD	2.33	0.58
2:D:329:LYS:HD2	2:D:333:LYS:HG3	1.85	0.58
2:B:329:LYS:HD2	2:B:333:LYS:HG3	1.85	0.58
2:C:329:LYS:HD2	2:C:333:LYS:HG3	1.85	0.57
2:A:361:ARG:O	2:A:362:PRO:C	2.43	0.57
2:B:643:LEU:O	2:B:647:MET:HG3	2.04	0.57
2:A:718:LEU:O	2:A:722:VAL:HG23	2.03	0.57
2:C:718:LEU:O	2:C:722:VAL:HG23	2.03	0.57
2:D:643:LEU:O	2:D:647:MET:HG3	2.05	0.57
2:A:329:LYS:HD2	2:A:333:LYS:HG3	1.85	0.57
2:C:292:LEU:HD22	2:C:295:ARG:NH2	2.20	0.56
2:A:643:LEU:O	2:A:647:MET:HG3	2.04	0.56
2:C:643:LEU:O	2:C:647:MET:HG3	2.05	0.56
2:B:34:THR:O	2:B:38:THR:HG23	2.06	0.55
2:D:34:THR:O	2:D:38:THR:HG23	2.06	0.55
2:D:723:ARG:C	2:D:725:GLU:H	2.14	0.55
1:4:1:A:P	1:4:5:A:O3'	2.65	0.55
2:A:34:THR:O	2:A:38:THR:HG23	2.06	0.54
2:C:34:THR:O	2:C:38:THR:HG23	2.06	0.54
2:D:404:VAL:HB	2:D:449:VAL:HG12	1.89	0.54
2:D:723:ARG:O	2:D:725:GLU:N	2.40	0.54
2:A:726:VAL:HG13	2:A:728:LEU:H	1.72	0.54
2:B:404:VAL:HB	2:B:449:VAL:HG12	1.90	0.54
2:A:404:VAL:HB	2:A:449:VAL:HG12	1.90	0.53
2:C:404:VAL:HB	2:C:449:VAL:HG12	1.90	0.53
1:4:3:A:C8	2:D:411:GLY:HA2	2.44	0.52
2:C:359:ARG:C	2:C:361:ARG:H	2.16	0.51
2:B:338:VAL:HA	2:B:343:LEU:HD12	1.93	0.50
2:B:726:VAL:HG12	2:B:729:THR:OG1	2.12	0.50
2:C:727:ARG:NH1	2:C:735:VAL:HG23	2.17	0.50
2:D:338:VAL:HA	2:D:343:LEU:HD12	1.93	0.50
2:B:53:GLY:O	2:B:54:LEU:HG	2.12	0.50
2:D:53:GLY:O	2:D:54:LEU:HG	2.12	0.50
2:A:53:GLY:O	2:A:54:LEU:HG	2.12	0.49
2:A:727:ARG:O	2:A:732:ASP:HA	2.13	0.49
2:C:53:GLY:O	2:C:54:LEU:HG	2.12	0.49
2:D:718:LEU:O	2:D:722:VAL:HG23	2.12	0.49
2:C:727:ARG:CZ	2:C:734:SER:HA	2.43	0.49
2:A:83:GLU:HG2	2:A:85:ARG:HG3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:326:LEU:H	2:D:327:PRO:HD3	1.78	0.49
2:B:83:GLU:HG2	2:B:85:ARG:HG3	1.95	0.49
2:B:325:ARG:O	2:B:326:LEU:HB2	2.13	0.49
2:C:83:GLU:HG2	2:C:85:ARG:HG3	1.95	0.49
2:D:83:GLU:HG2	2:D:85:ARG:HG3	1.95	0.49
2:B:326:LEU:H	2:B:327:PRO:HD3	1.78	0.49
2:D:325:ARG:O	2:D:326:LEU:HB2	2.13	0.49
2:A:338:VAL:HA	2:A:343:LEU:HD12	1.94	0.49
2:D:738:ALA:O	2:D:742:VAL:HG23	2.13	0.49
2:C:338:VAL:HA	2:C:343:LEU:HD12	1.94	0.49
2:A:724:ASN:HB3	2:A:730:HIS:HE1	1.78	0.48
2:B:738:ALA:O	2:B:742:VAL:HG23	2.13	0.48
2:A:738:ALA:O	2:A:742:VAL:HG23	2.13	0.48
2:C:738:ALA:O	2:C:742:VAL:HG23	2.13	0.48
2:C:325:ARG:O	2:C:326:LEU:HB2	2.13	0.48
2:A:325:ARG:O	2:A:326:LEU:HB2	2.13	0.48
1:1:5:A:OP1	2:A:176:MET:HG3	2.13	0.48
2:B:229:GLN:HE21	2:B:589:ALA:HA	1.79	0.48
2:B:723:ARG:O	2:B:725:GLU:N	2.47	0.48
2:D:229:GLN:HE21	2:D:589:ALA:HA	1.79	0.48
2:A:326:LEU:H	2:A:327:PRO:HD3	1.78	0.47
2:C:326:LEU:H	2:C:327:PRO:HD3	1.78	0.47
2:C:292:LEU:HD23	2:C:295:ARG:NH2	2.29	0.47
2:C:726:VAL:H	2:C:729:THR:HG1	1.62	0.47
2:D:727:ARG:H	2:D:727:ARG:HG3	1.32	0.47
2:A:229:GLN:HE21	2:A:589:ALA:HA	1.79	0.47
2:B:295:ARG:HD3	2:B:295:ARG:HA	1.57	0.47
2:C:229:GLN:HE21	2:C:589:ALA:HA	1.79	0.47
2:D:257:VAL:HG11	2:D:278:LEU:HD13	1.97	0.47
2:B:257:VAL:HG11	2:B:278:LEU:HD13	1.97	0.46
2:C:53:GLY:C	2:C:55:LEU:H	2.23	0.46
2:D:726:VAL:HG13	2:D:728:LEU:H	1.80	0.46
2:A:53:GLY:C	2:A:55:LEU:H	2.23	0.46
2:B:99:GLY:H	2:B:564:GLN:HB2	1.80	0.46
2:B:170:MET:HB2	2:B:194:LEU:HD11	1.97	0.46
2:A:99:GLY:H	2:A:564:GLN:HB2	1.80	0.46
2:B:53:GLY:C	2:B:55:LEU:H	2.23	0.46
2:D:727:ARG:O	2:D:732:ASP:HA	2.15	0.46
1:4:5:A:OP1	2:D:176:MET:HG3	2.15	0.46
2:B:726:VAL:H	2:B:729:THR:HB	1.80	0.46
2:D:53:GLY:C	2:D:55:LEU:H	2.23	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:ARG:H	2:D:165:PRO:HD2	1.80	0.46
2:D:170:MET:HB2	2:D:194:LEU:HD11	1.97	0.46
2:B:164:ARG:H	2:B:165:PRO:HD2	1.80	0.46
2:B:361:ARG:HB2	2:B:381:THR:HG21	1.97	0.46
2:C:47:THR:HG22	2:C:49:ALA:H	1.80	0.46
2:A:47:THR:HG22	2:A:49:ALA:H	1.80	0.46
2:C:164:ARG:H	2:C:165:PRO:HD2	1.80	0.46
2:C:292:LEU:HD22	2:C:295:ARG:HH21	1.81	0.46
2:A:164:ARG:H	2:A:165:PRO:HD2	1.80	0.45
2:A:359:ARG:HE	2:A:359:ARG:HB2	1.49	0.45
2:A:170:MET:HB2	2:A:194:LEU:HD11	1.97	0.45
2:B:330:GLU:HG3	2:B:332:GLY:H	1.82	0.45
2:D:330:GLU:HG3	2:D:332:GLY:H	1.82	0.45
2:D:724:ASN:ND2	2:D:724:ASN:H	2.14	0.45
2:C:170:MET:HB2	2:C:194:LEU:HD11	1.97	0.45
2:C:257:VAL:HG11	2:C:278:LEU:HD13	1.97	0.45
2:A:257:VAL:HG11	2:A:278:LEU:HD13	1.97	0.45
2:A:330:GLU:HG3	2:A:332:GLY:H	1.82	0.45
2:C:330:GLU:HG3	2:C:332:GLY:H	1.82	0.45
1:4:5:A:H62	2:D:561:GLN:H	1.63	0.45
2:B:726:VAL:O	2:B:727:ARG:C	2.59	0.45
2:D:47:THR:HG22	2:D:49:ALA:H	1.80	0.45
2:B:47:THR:HG22	2:B:49:ALA:H	1.80	0.45
2:B:166:VAL:HG11	2:B:185:VAL:HG21	1.99	0.44
1:2:5:A:OP1	2:B:176:MET:HG3	2.16	0.44
1:3:5:A:OP1	2:C:176:MET:HG3	2.17	0.44
2:A:361:ARG:HB2	2:A:381:THR:HG21	1.99	0.44
2:B:303:GLU:OE2	2:B:303:GLU:HA	2.18	0.44
2:D:303:GLU:OE2	2:D:303:GLU:HA	2.18	0.44
2:A:723:ARG:HE	2:A:724:ASN:ND2	2.16	0.44
2:B:726:VAL:HG13	2:B:727:ARG:N	2.31	0.44
2:B:723:ARG:C	2:B:725:GLU:H	2.26	0.44
2:D:726:VAL:O	2:D:729:THR:N	2.51	0.44
2:B:509:VAL:HG21	2:B:535:ALA:HA	1.99	0.43
2:C:644:LEU:O	2:C:648:GLU:HG3	2.18	0.43
2:D:166:VAL:HG11	2:D:185:VAL:HG21	2.00	0.43
2:D:509:VAL:HG21	2:D:535:ALA:HA	1.99	0.43
2:A:166:VAL:HG11	2:A:185:VAL:HG21	1.99	0.43
2:A:644:LEU:O	2:A:648:GLU:HG3	2.18	0.43
2:C:166:VAL:HG11	2:C:185:VAL:HG21	1.99	0.43
2:B:28:ALA:C	2:B:30:HIS:H	2.26	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:ALA:C	2:D:30:HIS:H	2.26	0.43
2:A:28:ALA:C	2:A:30:HIS:H	2.25	0.43
2:C:28:ALA:C	2:C:30:HIS:H	2.25	0.43
2:D:361:ARG:HA	2:D:361:ARG:HD3	1.60	0.43
2:A:303:GLU:HA	2:A:303:GLU:OE2	2.18	0.43
2:C:303:GLU:OE2	2:C:303:GLU:HA	2.18	0.43
2:C:509:VAL:HG21	2:C:535:ALA:HA	1.99	0.43
2:A:361:ARG:HD2	2:A:361:ARG:HA	1.65	0.43
2:C:780:ASP:O	2:C:784:GLU:HG3	2.19	0.43
2:A:509:VAL:HG21	2:A:535:ALA:HA	1.99	0.43
2:A:780:ASP:O	2:A:784:GLU:HG3	2.19	0.43
2:A:326:LEU:HG	2:A:329:LYS:HG3	2.01	0.42
2:C:326:LEU:HG	2:C:329:LYS:HG3	2.01	0.42
2:A:333:LYS:HA	2:A:333:LYS:HD3	1.78	0.42
2:C:113:LEU:HD12	2:C:113:LEU:HA	1.86	0.42
2:C:333:LYS:HA	2:C:333:LYS:HD3	1.78	0.42
2:A:611:ARG:HD3	2:A:611:ARG:HA	1.75	0.42
2:B:333:LYS:HA	2:B:333:LYS:HD3	1.78	0.42
2:D:644:LEU:O	2:D:648:GLU:HG3	2.18	0.42
2:B:644:LEU:O	2:B:648:GLU:HG3	2.18	0.42
2:C:660:ASP:HB2	2:C:727:ARG:NH1	2.27	0.42
2:A:113:LEU:HD12	2:A:113:LEU:HA	1.86	0.42
2:A:726:VAL:O	2:A:729:THR:N	2.52	0.42
2:D:780:ASP:O	2:D:784:GLU:HG3	2.19	0.42
2:B:326:LEU:HG	2:B:329:LYS:HG3	2.01	0.42
2:D:333:LYS:HA	2:D:333:LYS:HD3	1.78	0.42
2:B:780:ASP:O	2:B:784:GLU:HG3	2.19	0.42
2:C:611:ARG:HD3	2:C:611:ARG:HA	1.75	0.42
2:D:326:LEU:HG	2:D:329:LYS:HG3	2.01	0.42
2:B:360:LEU:HD23	2:B:360:LEU:HA	1.84	0.41
2:C:361:ARG:HD3	2:C:361:ARG:HA	1.46	0.41
2:D:275:LEU:HB3	2:D:297:TRP:HB2	2.03	0.41
2:A:176:MET:HE1	2:A:560:VAL:HG22	2.03	0.41
2:B:275:LEU:HB3	2:B:297:TRP:HB2	2.03	0.41
2:C:54:LEU:HD13	2:C:59:ALA:HB2	2.03	0.41
2:B:54:LEU:HD13	2:B:59:ALA:HB2	2.03	0.41
2:D:54:LEU:HD13	2:D:59:ALA:HB2	2.03	0.41
2:A:54:LEU:HD13	2:A:59:ALA:HB2	2.03	0.41
2:A:275:LEU:HB3	2:A:297:TRP:HB2	2.03	0.41
2:B:726:VAL:O	2:B:729:THR:N	2.53	0.41
2:C:275:LEU:HB3	2:C:297:TRP:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:721:GLU:HA	2:D:724:ASN:ND2	2.35	0.41
2:B:721:GLU:HA	2:B:724:ASN:HD22	1.84	0.41
2:C:729:THR:O	2:C:730:HIS:C	2.62	0.40
2:A:731:GLY:O	2:A:732:ASP:OD1	2.39	0.40
2:D:176:MET:HE1	2:D:560:VAL:HG22	2.02	0.40
2:C:576:ILE:H	2:C:576:ILE:HG12	1.75	0.40
2:D:357:GLY:O	2:D:362:PRO:HD3	2.21	0.40
2:D:723:ARG:C	2:D:725:GLU:N	2.79	0.40
2:A:200:PRO:HD3	2:A:499:PHE:HD2	1.87	0.40
2:A:512:ILE:O	2:A:516:VAL:HG23	2.22	0.40
2:A:576:ILE:H	2:A:576:ILE:HG12	1.74	0.40
2:C:200:PRO:HD3	2:C:499:PHE:HD2	1.87	0.40
2:C:512:ILE:O	2:C:516:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	777/797 (98%)	738 (95%)	32 (4%)	7 (1%)	14	31
2	B	777/797 (98%)	736 (95%)	33 (4%)	8 (1%)	12	28
2	C	777/797 (98%)	741 (95%)	31 (4%)	5 (1%)	21	41
2	D	777/797 (98%)	741 (95%)	30 (4%)	6 (1%)	16	34
All	All	3108/3188 (98%)	2956 (95%)	126 (4%)	26 (1%)	18	34

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	326	LEU
2	A	725	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	326	LEU
2	C	326	LEU
2	C	361	ARG
2	D	326	LEU
2	D	724	ASN
2	A	361	ARG
2	B	724	ASN
2	B	731	GLY
2	B	732	ASP
2	A	164	ARG
2	A	724	ASN
2	B	164	ARG
2	B	361	ARG
2	C	164	ARG
2	D	164	ARG
2	A	149	ASP
2	B	149	ASP
2	C	149	ASP
2	D	149	ASP
2	A	41	VAL
2	B	41	VAL
2	C	41	VAL
2	D	41	VAL
2	D	361	ARG

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 PDB entries followed by that with respect to all EM entries.

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	597/607 (98%)	582 (98%)	15 (2%)	42	69
2	B	597/607 (98%)	584 (98%)	13 (2%)	45	72
2	C	597/607 (98%)	585 (98%)	12 (2%)	48	74
2	D	597/607 (98%)	582 (98%)	15 (2%)	42	69
All	All	2388/2428 (98%)	2333 (98%)	55 (2%)	44	71

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	149	ASP
2	A	257	VAL
2	A	270	VAL
2	A	359	ARG
2	A	361	ARG
2	A	370	ASP
2	A	597	LEU
2	A	600	LEU
2	A	725	GLU
2	A	726	VAL
2	A	727	ARG
2	A	728	LEU
2	A	729	THR
2	A	737	GLU
2	A	762	ARG
2	B	149	ASP
2	B	257	VAL
2	B	270	VAL
2	B	295	ARG
2	B	359	ARG
2	B	361	ARG
2	B	597	LEU
2	B	600	LEU
2	B	726	VAL
2	B	729	THR
2	B	732	ASP
2	B	737	GLU
2	B	762	ARG
2	C	100	ASP
2	C	149	ASP
2	C	257	VAL
2	C	270	VAL
2	C	359	ARG
2	C	361	ARG
2	C	370	ASP
2	C	597	LEU
2	C	600	LEU
2	C	728	LEU
2	C	737	GLU
2	C	762	ARG
2	D	149	ASP
2	D	257	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	270	VAL
2	D	359	ARG
2	D	597	LEU
2	D	600	LEU
2	D	723	ARG
2	D	724	ASN
2	D	725	GLU
2	D	726	VAL
2	D	727	ARG
2	D	728	LEU
2	D	729	THR
2	D	737	GLU
2	D	762	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	237	HIS
2	A	251	GLN
2	A	274	GLN
2	A	345	GLN
2	A	401	GLN
2	A	532	GLN
2	A	550	HIS
2	A	724	ASN
2	A	745	ASN
2	B	237	HIS
2	B	251	GLN
2	B	274	GLN
2	B	397	HIS
2	B	401	GLN
2	B	532	GLN
2	B	550	HIS
2	B	724	ASN
2	B	745	ASN
2	C	237	HIS
2	C	251	GLN
2	C	274	GLN
2	C	345	GLN
2	C	401	GLN
2	C	532	GLN
2	C	550	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	745	ASN
2	D	237	HIS
2	D	251	GLN
2	D	274	GLN
2	D	345	GLN
2	D	397	HIS
2	D	401	GLN
2	D	532	GLN
2	D	550	HIS
2	D	724	ASN
2	D	730	HIS
2	D	745	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	4/5 (80%)	4 (100%)	1 (25%)
1	2	4/5 (80%)	4 (100%)	1 (25%)
1	3	4/5 (80%)	4 (100%)	1 (25%)
1	4	4/5 (80%)	4 (100%)	0
All	All	16/20 (80%)	16 (100%)	3 (18%)

All (16) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	A
1	1	3	A
1	1	4	A
1	1	5	A
1	2	2	A
1	2	3	A
1	2	4	A
1	2	5	A
1	3	2	A
1	3	3	A
1	3	4	A
1	3	5	A
1	4	2	A
1	4	3	A
1	4	4	A
1	4	5	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	3	A
1	2	3	A
1	3	3	A

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.