



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 11:53 PM UTC

PDB ID : 6OEM / pdb_00006oem
EMDB ID : EMD-20030
Title : Cryo-EM structure of mouse RAG1/2 PRC complex (DNA0)
Authors : Chen, X.; Cui, Y.; Zhou, Z.H.; Yang, W.; Gellert, M.
Deposited on : 2019-03-27
Resolution : 3.60 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 : 0.0.1.dev132
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

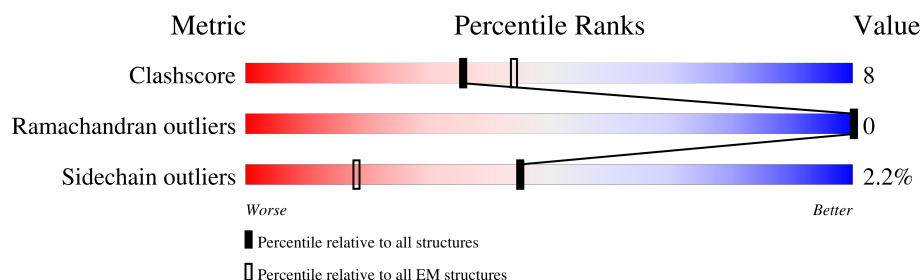
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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

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	A	1040	46% 12% • 42%
1	C	1040	46% 12% • 41%
2	B	527	56% 10% 34%
2	D	527	54% 12% 34%
3	G	61	38% 56% 7%
4	I	50	32% 60% 8%
5	F	50	32% 60% 8%
6	J	61	52% 41% 7%
7	H	141	38% • 61%

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Mol	Chain	Length	Quality of chain
7	N	141	23% 74%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19707 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 protein called V(D)J recombination-activating protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	606	Total	C	N	O	S	0	0
			4774	3010	846	885	33		
1	C	611	Total	C	N	O	S	0	0
			4843	3053	856	901	33		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	962	GLN	GLU	engineered mutation	UNP P15919
C	962	GLN	GLU	engineered mutation	UNP P15919

- Molecule 2 is a protein called V(D)J recombination-activating protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	346	Total	C	N	O	S	0	0
			2668	1706	454	490	18		
2	D	346	Total	C	N	O	S	0	0
			2671	1708	454	490	19		

- Molecule 3 is a DNA chain called DNA (57-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	57	Total	C	N	O	P	0	0
			1163	557	202	348	56		

- Molecule 4 is a DNA chain called DNA (46-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	46	Total	C	N	O	P	0	0
			936	446	172	272	46		

- Molecule 5 is a DNA chain called DNA (46-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	46	Total	C	N	O	P	0	0
			947	452	172	278	45		

- Molecule 6 is a DNA chain called DNA (57-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	57	Total	C	N	O	P	0	0
			1171	556	224	334	57		

- Molecule 7 is a protein called High mobility group protein B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	36	Total	C	N	O	S	0	0
			242	157	41	42	2		
7	H	55	Total	C	N	O	S	0	0
			288	174	55	58	1		

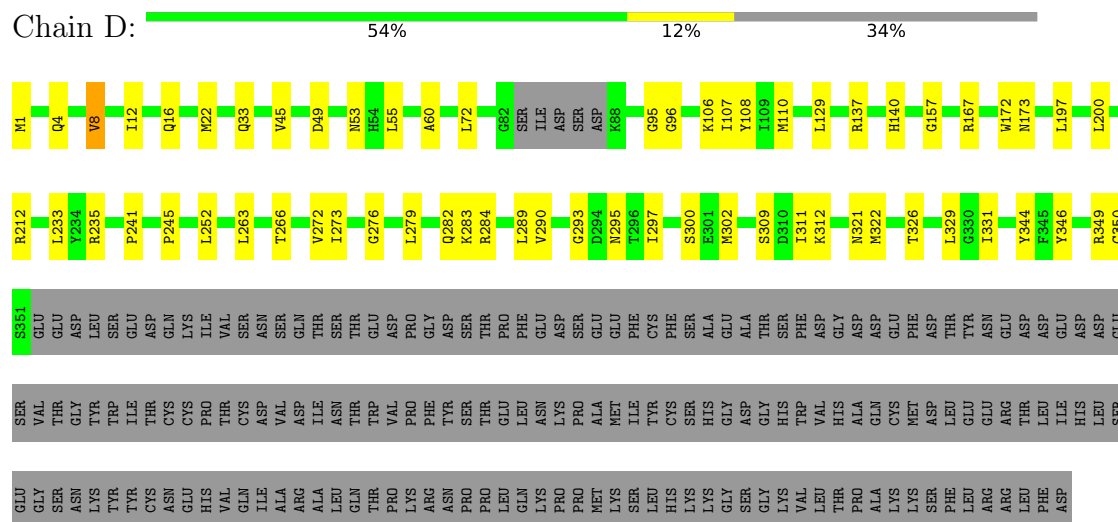
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Mg	0
			1	1	
8	C	1	Total	Mg	0
			1	1	

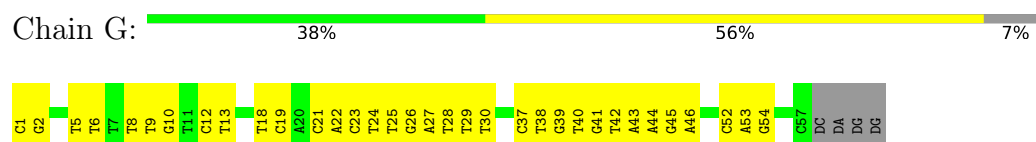
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	Zn	0
			1	1	
9	C	1	Total	Zn	0
			1	1	

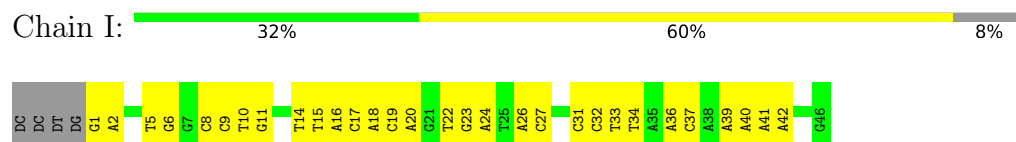
- Molecule 2: V(D)J recombination-activating protein 2



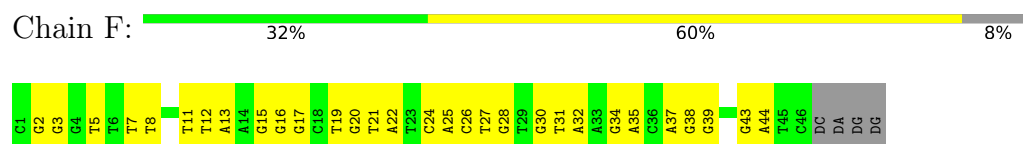
- Molecule 3: DNA (57-MER)



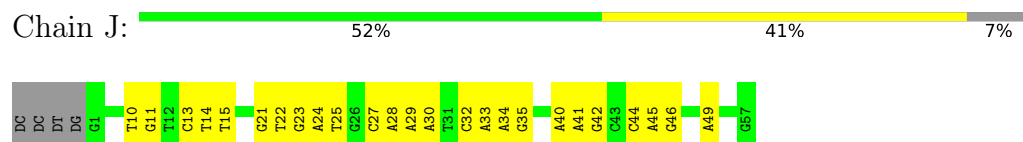
- Molecule 4: DNA (46-MER)



- Molecule 5: DNA (46-MER)



- Molecule 6: DNA (57-MER)



- Molecule 7: High mobility group protein B1



SER TYR ALA PHE PHE VAL GLN THR CYS ARG GLU GLU HIS LYS LYS LYS HIS PRO PRO ASP ALA ALA VAL ASN PHE SER GLU PHE SER LYS CYS SER GLU ARG TRP LYS THR MET SER ALA LYS GLU LYS GLY LYS PHE GLU TYR GLU ASP MET ALA LYS ASP LYS ALA ARG TYR GLU ARG GLU

MET LYS THR TYR ILE PRO PRO LYS GLY THR LYS LYS LYS PHE LYS ASP PRO ASN ALA ALA ARG LYS PRO P99 R110 P111 G119 LEU SER I172 L129 M132 T1136 ALA ALA ASP ASP LYS GLN PRO TYR GLU ASP LYS LYS ALA LYS LEU LYS GLU LYS TYR

● Molecule 7: High mobility group protein B1



SER TYR ALA PHE PHE VAL GLN THR CYS ARG GLU GLU HIS LYS LYS LYS HIS PRO PRO ASP ALA ALA VAL ASN PHE SER GLU PHE SER LYS CYS SER GLU ARG TRP LYS THR MET SER ALA LYS GLU LYS GLY LYS PHE GLU TYR GLU ASP MET ALA LYS ASP LYS ALA ARG TYR GLU ARG GLU

MET LYS THR TYR ILE PRO PRO LYS GLY THR LYS LYS LYS PHE LYS ASP PRO ASN ALA ALA ARG LYS PRO SER A103 S107 Y155

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109865	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.11	0/4873	0.30	0/6581
1	C	0.12	0/4942	0.29	0/6667
2	B	0.09	0/2736	0.26	0/3713
2	D	0.10	0/2739	0.26	0/3716
3	G	0.17	0/1301	0.37	0/2007
4	I	0.15	0/1049	0.29	0/1614
5	F	0.17	0/1062	0.37	0/1640
6	J	0.15	0/1316	0.31	0/2028
7	H	0.07	0/290	0.22	0/403
7	N	0.08	0/250	0.21	0/339
All	All	0.12	0/20558	0.30	0/28708

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

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	4774	0	4673	78	0
1	C	4843	0	4770	78	0
2	B	2668	0	2602	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2671	0	2609	33	0
3	G	1163	0	648	22	0
4	I	936	0	517	24	0
5	F	947	0	522	22	0
6	J	1171	0	639	22	0
7	H	288	0	178	1	0
7	N	242	0	183	2	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
All	All	19707	0	17341	288	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 8.

All (288) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:CYS:O	1:A:908:GLN:HG2	1.50	1.11
1:A:907:CYS:O	1:A:908:GLN:CG	2.28	0.82
5:F:7:DT:H2''	5:F:8:DT:H5''	1.71	0.72
1:A:983:GLU:HG3	1:A:984:MET:N	2.08	0.68
1:C:471:ARG:NH2	1:C:478:CYS:SG	2.67	0.68
1:A:428:LYS:HB2	1:C:442:ARG:HH12	1.60	0.67
1:C:518:GLU:HG3	1:C:688:THR:HB	1.77	0.66
3:G:9:DT:H2''	3:G:10:DG:H5''	1.77	0.66
1:A:629:ILE:HB	1:A:641:PHE:HB3	1.77	0.65
2:B:283:LYS:NZ	2:B:311:ILE:O	2.29	0.65
1:A:846:ILE:HG13	1:A:848:ARG:H	1.62	0.65
1:C:420:ASP:HA	1:C:425:GLY:H	1.61	0.65
1:C:432:LEU:HD21	1:C:455:MET:HE2	1.79	0.64
2:D:283:LYS:NZ	2:D:311:ILE:O	2.31	0.64
1:A:607:GLU:HG2	1:A:973:LYS:HD3	1.78	0.64
4:I:42:DA:H61	5:F:5:DT:H3	1.43	0.64
1:C:713:ARG:NH2	1:C:726:ILE:O	2.29	0.64
1:A:907:CYS:C	1:A:908:GLN:HG2	2.23	0.62
1:C:607:GLU:HG2	1:C:607:GLU:O	1.98	0.62
1:A:588:ASN:HD22	1:A:589:GLY:H	1.46	0.61
1:A:724:VAL:HG22	1:A:734:ARG:H	1.65	0.61
5:F:15:DG:H2''	5:F:16:DG:H5''	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:ARG:HD3	1:A:931:LYS:HA	1.83	0.61
1:C:691:MET:HE3	1:C:696:ARG:HG3	1.82	0.60
1:C:761:ARG:NH2	2:D:108:TYR:OH	2.35	0.60
1:A:864:ASP:OD1	1:A:880:ARG:NH1	2.35	0.59
4:I:8:DC:H2''	4:I:9:DC:H5''	1.85	0.59
1:A:546:ASP:OD1	2:B:260:SER:OG	2.21	0.59
2:B:263:LEU:O	2:B:321:ASN:ND2	2.35	0.59
1:A:773:ARG:HD3	2:B:39:ARG:HH12	1.69	0.58
2:D:1:MET:N	2:D:349:ARG:O	2.36	0.58
3:G:42:DT:H2''	3:G:43:DA:C8	2.39	0.58
1:A:521:PRO:HG2	1:A:685:SER:HA	1.83	0.58
1:A:419:ALA:O	1:A:424:GLY:N	2.36	0.58
5:F:27:DT:H2'	5:F:28:DG:C8	2.38	0.57
1:A:969:ARG:NH1	5:F:30:DG:OP1	2.36	0.57
5:F:37:DA:H2''	5:F:38:DG:H5''	1.86	0.57
1:A:547:GLU:OE2	2:B:159:ARG:NH1	2.37	0.57
1:C:469:ALA:O	1:C:473:ASN:ND2	2.37	0.57
1:C:694:ILE:HD11	1:C:696:ARG:HH21	1.70	0.57
2:D:266:THR:OG1	2:D:350:CYS:SG	2.61	0.57
5:F:24:DC:H2''	5:F:25:DA:C8	2.40	0.57
4:I:22:DT:H2''	4:I:23:DG:C8	2.39	0.57
1:C:719:GLU:OE1	1:C:722:GLY:N	2.38	0.57
5:F:16:DG:H2'	5:F:17:DG:C8	2.40	0.57
2:B:16:GLN:NE2	2:B:33:GLN:O	2.37	0.56
1:A:734:ARG:NH1	1:A:932:ILE:O	2.38	0.56
1:A:595:VAL:HG22	1:A:626:VAL:HG22	1.88	0.56
1:C:597:GLU:HB3	1:C:704:GLY:HA2	1.87	0.56
1:C:724:VAL:HG12	1:C:734:ARG:H	1.71	0.55
2:B:22:MET:HE1	2:B:110:MET:HG2	1.88	0.55
2:D:4:GLN:NE2	2:D:53:ASN:OD1	2.39	0.55
5:F:20:DG:H2''	5:F:21:DT:H5''	1.88	0.55
2:D:16:GLN:NE2	2:D:33:GLN:O	2.39	0.55
6:J:34:DA:H2'	6:J:35:DG:H8	1.71	0.55
1:A:789:PRO:O	1:A:949:ARG:NH2	2.40	0.55
2:D:22:MET:HE1	2:D:110:MET:HG2	1.89	0.55
1:A:628:ARG:NH1	1:A:642:GLU:OE2	2.40	0.54
1:C:867:CYS:O	1:C:876:HIS:NE2	2.39	0.54
1:C:908:GLN:O	1:C:912:ASN:ND2	2.39	0.54
1:C:596:LYS:HB2	1:C:627:MET:HE3	1.88	0.54
1:A:446:ARG:NH2	5:F:19:DT:OP1	2.41	0.54
1:A:518:GLU:HG3	1:A:688:THR:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:989:LYS:NZ	4:I:24:DA:OP1	2.40	0.54
5:F:31:DT:H2''	5:F:32:DA:N7	2.22	0.54
1:C:814:GLU:O	1:C:818:HIS:ND1	2.39	0.54
2:D:331:ILE:O	2:D:344:TYR:N	2.39	0.54
3:G:38:DT:H2''	3:G:39:DG:C8	2.43	0.54
1:A:980:LYS:NZ	3:G:39:DG:OP1	2.41	0.54
1:C:716:GLU:OE2	1:C:753:ASN:ND2	2.40	0.54
1:A:462:LEU:HD12	1:A:466:VAL:HB	1.90	0.54
6:J:24:DA:H2''	6:J:25:DT:H5''	1.88	0.54
6:J:40:DA:H2'	6:J:41:DA:H8	1.73	0.53
1:C:594:VAL:HB	1:C:628:ARG:HG2	1.90	0.53
2:D:137:ARG:HH11	2:D:157:GLY:HA3	1.74	0.53
6:J:27:DC:H2''	6:J:28:DA:C8	2.43	0.53
1:A:797:ASP:OD1	1:A:893:TRP:NE1	2.41	0.53
6:J:41:DA:H2'	6:J:42:DG:C8	2.44	0.53
4:I:18:DA:H2''	4:I:19:DC:H5''	1.91	0.53
2:D:197:LEU:HB2	2:D:200:LEU:HD23	1.90	0.53
6:J:34:DA:H2'	6:J:35:DG:C8	2.44	0.53
3:G:40:DT:H2''	3:G:41:DG:N7	2.24	0.52
1:A:979:SER:HB2	3:G:37:DC:H4'	1.92	0.52
1:C:658:MET:SD	1:C:658:MET:N	2.83	0.52
2:B:241:PRO:HD2	2:B:245:PRO:HA	1.92	0.52
1:C:837:LEU:HD21	1:C:843:LEU:HB3	1.92	0.52
6:J:44:DC:H2''	6:J:45:DA:C8	2.45	0.52
3:G:12:DC:H2''	3:G:13:DT:H5'	1.92	0.52
1:A:962:GLN:NE2	4:I:20:DA:OP1	2.39	0.51
1:C:521:PRO:HG2	1:C:685:SER:HA	1.90	0.51
1:C:969:ARG:NH1	3:G:41:DG:OP1	2.43	0.51
2:B:95:GLY:HA3	2:B:140:HIS:HE1	1.74	0.51
1:C:863:VAL:HA	1:C:866:VAL:HG22	1.92	0.51
1:A:400:THR:OG1	1:A:401:ARG:N	2.43	0.51
1:A:873:GLU:OE1	1:A:873:GLU:N	2.43	0.51
1:C:703:ARG:NH2	1:C:950:ASP:OD1	2.44	0.51
6:J:45:DA:H2'	6:J:46:DG:C8	2.46	0.51
1:C:983:GLU:HG2	1:C:984:MET:N	2.26	0.51
1:A:536:ASP:OD1	1:A:555:LYS:NZ	2.43	0.50
1:A:716:GLU:OE2	1:A:787:THR:OG1	2.30	0.50
2:B:142:ILE:HD12	2:B:155:LEU:HD12	1.93	0.50
1:C:978:GLN:HB3	5:F:27:DT:H1'	1.94	0.50
4:I:41:DA:H2'	4:I:42:DA:C8	2.46	0.50
1:A:717:GLY:HA2	1:A:781:ALA:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:810:LEU:HD13	1:C:815:VAL:HG21	1.92	0.50
5:F:21:DT:H2''	5:F:22:DA:H8	1.76	0.50
2:D:263:LEU:O	2:D:321:ASN:ND2	2.45	0.50
1:C:909:TYR:HA	1:C:912:ASN:HD21	1.76	0.49
1:C:647:ASN:ND2	1:C:955:ALA:O	2.46	0.49
3:G:23:DC:H2''	3:G:24:DT:H5'	1.94	0.49
1:C:744:HIS:CD2	1:C:937:HIS:HE1	2.30	0.49
5:F:13:DA:H2''	7:H:107:SER:HA	1.94	0.49
1:A:571:GLU:HG2	1:A:691:MET:HE3	1.93	0.49
1:A:471:ARG:NH1	1:A:478:CYS:SG	2.79	0.49
3:G:29:DT:H4'	3:G:30:DT:OP1	2.12	0.49
1:C:870:ILE:HD12	1:C:871:PRO:HD2	1.94	0.49
1:A:546:ASP:OD2	2:B:259:SER:OG	2.28	0.49
1:C:511:LEU:HD21	1:C:989:LYS:HG3	1.94	0.49
1:C:760:TRP:HB2	1:C:776:VAL:HG11	1.95	0.49
2:B:212:ARG:NH1	2:B:293:GLY:O	2.45	0.49
1:C:920:LEU:HD22	1:C:924:PHE:HB2	1.95	0.49
2:B:72:LEU:HD13	2:B:96:GLY:HA3	1.94	0.49
1:A:703:ARG:NH2	1:A:950:ASP:OD1	2.46	0.49
1:C:633:HIS:ND1	1:C:633:HIS:O	2.45	0.49
4:I:31:DC:H2''	4:I:32:DC:H5'	1.95	0.49
1:C:709:GLU:HA	1:C:712:VAL:HG12	1.94	0.48
2:D:276:GLY:H	2:D:284:ARG:HD3	1.76	0.48
5:F:25:DA:H2''	5:F:26:DC:H5''	1.95	0.48
2:B:49:ASP:OD1	2:B:49:ASP:N	2.44	0.48
5:F:21:DT:H2''	5:F:22:DA:C8	2.49	0.48
1:A:837:LEU:HB3	1:A:843:LEU:HD21	1.96	0.48
1:C:639:LYS:HD3	1:C:642:GLU:HB2	1.95	0.48
1:C:717:GLY:HA2	1:C:781:ALA:HB3	1.93	0.48
1:C:418:PHE:HA	1:C:421:LYS:HG2	1.96	0.48
3:G:52:DC:H2'	3:G:53:DA:C8	2.49	0.48
1:C:726:ILE:HB	1:C:934:ASN:HB3	1.95	0.48
1:C:515:HIS:CD2	1:C:568:MET:HE2	2.48	0.48
1:A:984:MET:HA	1:A:987:VAL:HG12	1.95	0.48
2:D:289:LEU:N	2:D:300:SER:O	2.33	0.48
3:G:5:DT:H2''	3:G:6:DT:H5''	1.94	0.48
1:A:606:SER:OG	1:A:617:GLU:OE1	2.31	0.48
1:A:657:LEU:HD23	1:A:988:LEU:HD23	1.94	0.48
6:J:10:DT:H2''	6:J:11:DG:N7	2.29	0.48
5:F:2:DG:H2''	5:F:3:DG:C8	2.48	0.48
1:A:594:VAL:HB	1:A:628:ARG:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:19:DC:H2''	4:I:20:DA:H8	1.80	0.47
1:C:469:ALA:HA	1:C:999:LEU:HD23	1.97	0.47
2:B:141:SER:HG	2:B:207:HIS:HE2	1.61	0.47
3:G:53:DA:H2''	3:G:54:DG:C8	2.49	0.47
6:J:40:DA:H2'	6:J:41:DA:C8	2.49	0.47
1:A:476:LEU:HD22	1:A:481:TYR:HB2	1.96	0.47
1:A:563:LEU:HD21	1:A:700:PHE:CZ	2.50	0.47
2:D:45:VAL:HG23	2:D:60:ALA:HB3	1.95	0.47
2:B:309:SER:HA	2:B:312:LYS:HZ2	1.80	0.47
1:A:841:MET:HB3	1:A:843:LEU:HD22	1.97	0.47
4:I:15:DT:H2''	4:I:16:DA:C8	2.50	0.47
1:A:708:ASP:OD1	1:A:708:ASP:N	2.45	0.46
3:G:27:DA:H2'	3:G:28:DT:H71	1.97	0.46
2:B:279:LEU:HB2	2:B:282:GLN:HG3	1.97	0.46
1:A:534:ILE:HD12	1:A:985:GLU:HB3	1.98	0.46
4:I:40:DA:H2'	4:I:41:DA:C8	2.51	0.46
4:I:39:DA:H2'	4:I:40:DA:C8	2.51	0.46
1:A:718:LEU:HD11	1:A:748:ARG:HH22	1.80	0.46
4:I:33:DT:C6	4:I:34:DT:H73	2.51	0.46
6:J:21:DG:H2'	6:J:22:DT:C6	2.50	0.46
1:A:567:LEU:O	1:A:571:GLU:HG3	2.16	0.46
2:D:72:LEU:HD13	2:D:96:GLY:HA3	1.96	0.46
2:D:241:PRO:HD2	2:D:245:PRO:HA	1.98	0.46
3:G:21:DC:H2''	3:G:22:DA:H5'	1.98	0.46
2:B:272:VAL:HG23	2:B:289:LEU:HG	1.97	0.45
1:A:909:TYR:OH	1:A:939:THR:O	2.35	0.45
3:G:9:DT:H3	6:J:49:DA:H2	1.63	0.45
1:A:407:ARG:NH1	1:C:423:GLU:OE2	2.49	0.45
1:A:740:ASN:HB3	1:A:743:PHE:CD2	2.51	0.45
2:B:45:VAL:HG23	2:B:60:ALA:HB3	1.97	0.45
3:G:8:DT:H2''	3:G:9:DT:H5'	1.99	0.45
7:N:129:LEU:HA	7:N:132:MET:HE2	1.97	0.45
4:I:14:DT:H2''	4:I:15:DT:H5''	1.99	0.45
6:J:41:DA:H2'	6:J:42:DG:H8	1.81	0.45
1:A:977:ARG:HD3	6:J:23:DG:H1'	1.99	0.45
6:J:14:DT:H4'	6:J:15:DT:OP1	2.16	0.45
6:J:45:DA:H2'	6:J:46:DG:H8	1.82	0.45
2:D:322:MET:HB2	2:D:326:THR:HB	1.99	0.45
3:G:25:DT:H4'	3:G:26:DG:OP1	2.16	0.45
1:A:863:VAL:HA	1:A:866:VAL:HG12	1.98	0.45
1:C:694:ILE:HG13	1:C:696:ARG:HE	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:45:DG:H2''	3:G:46:DA:C8	2.52	0.45
1:A:867:CYS:HG	1:A:876:HIS:CE1	2.27	0.45
2:B:288:SER:HA	2:B:301:GLU:HA	1.99	0.45
2:D:235:ARG:NH2	2:D:295:ASN:OD1	2.50	0.45
2:D:272:VAL:HG23	2:D:289:LEU:HG	1.99	0.45
1:C:708:ASP:OD1	1:C:708:ASP:N	2.50	0.44
2:D:95:GLY:HA3	2:D:140:HIS:HE1	1.82	0.44
2:D:233:LEU:HD11	2:D:252:LEU:HB2	1.98	0.44
1:C:984:MET:HA	1:C:987:VAL:HG12	1.99	0.44
2:B:266:THR:OG1	2:B:350:CYS:SG	2.63	0.44
1:A:507:GLU:HG3	1:A:993:LEU:HD11	2.00	0.44
2:D:289:LEU:HD11	2:D:302:MET:HB3	1.98	0.44
4:I:17:DC:H2''	4:I:18:DA:C8	2.53	0.44
1:C:761:ARG:NH2	2:D:106:LYS:HD3	2.33	0.44
2:B:4:GLN:NE2	2:B:53:ASN:OD1	2.51	0.44
2:D:49:ASP:OD1	2:D:49:ASP:N	2.51	0.44
1:A:607:GLU:O	1:A:609:HIS:ND1	2.48	0.44
5:F:34:DG:H1'	5:F:35:DA:C8	2.53	0.44
2:B:208:VAL:HB	2:B:219:LEU:HB2	1.99	0.44
4:I:19:DC:H2''	4:I:20:DA:C8	2.53	0.44
2:D:8:VAL:HG11	2:D:12:ILE:HG13	2.00	0.44
3:G:18:DT:H2''	3:G:19:DC:C5	2.52	0.44
1:A:810:LEU:HD12	1:A:815:VAL:HG21	1.99	0.43
6:J:32:DC:H2''	6:J:33:DA:N7	2.33	0.43
1:C:727:CYS:HB3	1:C:730:CYS:SG	2.56	0.43
2:D:167:ARG:NH2	2:D:172:TRP:O	2.42	0.43
6:J:22:DT:H2'	6:J:23:DG:C8	2.53	0.43
6:J:10:DT:H2''	6:J:11:DG:C8	2.53	0.43
1:C:588:ASN:ND2	1:C:695:PRO:O	2.51	0.43
1:A:730:CYS:SG	1:A:942:HIS:CE1	3.12	0.43
1:C:558:ARG:NH1	1:C:560:ASP:OD2	2.52	0.43
2:D:212:ARG:NH1	2:D:293:GLY:O	2.52	0.43
4:I:10:DT:H2''	4:I:11:DG:C8	2.53	0.43
1:A:467:CYS:O	1:A:470:ILE:HG13	2.17	0.43
1:C:538:LEU:O	2:D:173:ASN:ND2	2.47	0.43
1:C:541:LEU:HD13	1:C:542:ALA:H	1.83	0.43
1:A:907:CYS:SG	1:A:908:GLN:N	2.91	0.43
1:C:846:ILE:HG13	1:C:848:ARG:H	1.84	0.43
1:A:741:LEU:HB3	1:A:940:LEU:HD23	2.01	0.43
1:C:413:ILE:O	1:C:416:LYS:HG3	2.18	0.43
1:C:795:HIS:O	1:C:798:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:32:DC:H2''	4:I:33:DT:C6	2.54	0.43
5:F:43:DG:H2''	5:F:44:DA:C8	2.54	0.43
5:F:38:DG:H2''	5:F:39:DG:H5'	2.00	0.43
1:A:971:PHE:HB3	1:A:987:VAL:HG23	2.00	0.42
1:C:556:ARG:HH12	1:C:674:PRO:HB2	1.84	0.42
6:J:32:DC:H2''	6:J:33:DA:C8	2.54	0.42
4:I:40:DA:H2'	4:I:41:DA:H8	1.85	0.42
1:A:632:GLU:HA	1:A:637:ASN:HA	2.02	0.42
1:C:816:TYR:CD1	1:C:817:LYS:HG3	2.55	0.42
5:F:11:DT:H2''	5:F:12:DT:C6	2.53	0.42
1:A:451:LEU:HA	1:A:454:ILE:HG22	2.02	0.42
1:C:870:ILE:O	1:C:876:HIS:NE2	2.53	0.42
1:C:979:SER:HB2	5:F:26:DC:H4'	2.02	0.42
2:B:235:ARG:NH2	2:B:295:ASN:OD1	2.52	0.42
2:D:329:LEU:HD21	2:D:346:TYR:HB2	2.00	0.42
1:C:436:LEU:HD11	1:C:451:LEU:HD22	2.01	0.42
1:C:715:VAL:HG21	1:C:785:ILE:HD12	2.02	0.42
1:A:435:PHE:HE1	1:C:432:LEU:HA	1.84	0.42
1:A:731:ASP:HB3	1:A:748:ARG:HD3	2.01	0.42
1:C:538:LEU:HD13	1:C:541:LEU:HG	2.00	0.42
1:C:804:PHE:HD1	1:C:807:ILE:HD12	1.85	0.42
2:D:309:SER:HA	2:D:312:LYS:HZ2	1.85	0.42
2:B:311:ILE:HG12	2:B:331:ILE:HG13	2.01	0.42
2:D:107:ILE:HG13	2:D:129:LEU:HD11	2.02	0.42
4:I:1:DG:H2''	4:I:2:DA:C8	2.54	0.42
4:I:5:DT:H2''	4:I:6:DG:N7	2.35	0.42
1:A:768:SER:HB2	1:A:771:GLU:HG3	2.02	0.42
2:B:275:GLY:N	2:B:287:CYS:SG	2.93	0.41
3:G:1:DC:H2''	3:G:2:DG:C8	2.54	0.41
1:A:665:HIS:CD2	2:B:36:TRP:HE1	2.38	0.41
1:A:810:LEU:HD13	1:A:815:VAL:HG11	2.02	0.41
2:B:76:ALA:HB1	2:B:142:ILE:HG22	2.02	0.41
1:A:589:GLY:HA3	1:A:590:PRO:HA	1.88	0.41
1:A:710:LYS:HE2	1:A:710:LYS:HB3	1.92	0.41
2:B:263:LEU:HD23	2:B:273:ILE:HD13	2.02	0.41
2:B:333:GLY:H	2:B:342:ALA:C	2.28	0.41
1:C:972:ARG:O	1:C:972:ARG:HG3	2.20	0.41
1:A:505:ASN:O	1:A:508:LYS:HG3	2.21	0.41
1:C:971:PHE:HB3	1:C:987:VAL:HG23	2.03	0.41
1:A:469:ALA:O	1:A:473:ASN:ND2	2.53	0.41
1:A:568:MET:HE3	1:A:568:MET:HB2	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:LEU:O	1:C:404:GLN:NE2	2.53	0.41
1:C:740:ASN:HD21	1:C:743:PHE:HB2	1.85	0.41
6:J:13:DC:C6	6:J:14:DT:H72	2.56	0.41
1:A:566:ALA:HA	1:A:569:ASP:OD2	2.21	0.41
1:C:629:ILE:HB	1:C:641:PHE:HB3	2.01	0.41
4:I:26:DA:H2"	4:I:27:DC:H5"	2.02	0.41
1:C:719:GLU:OE1	1:C:721:SER:N	2.54	0.41
2:D:279:LEU:HB2	2:D:282:GLN:HG3	2.03	0.41
1:A:724:VAL:HG22	1:A:733:THR:HB	2.03	0.40
1:C:729:LEU:HB3	1:C:746:ILE:HG12	2.03	0.40
2:D:263:LEU:HD23	2:D:273:ILE:HD13	2.02	0.40
3:G:43:DA:H2"	3:G:44:DA:C8	2.57	0.40
6:J:29:DA:H2"	6:J:30:DA:C8	2.57	0.40
1:C:737:ALA:HB3	1:C:932:ILE:HG21	2.03	0.40
1:C:482:HIS:HB2	1:C:500:LEU:HD21	2.04	0.40
1:C:669:THR:HG22	1:C:784:PHE:CZ	2.57	0.40
4:I:36:DA:H2"	4:I:37:DC:H5"	2.02	0.40
7:N:110:ARG:N	7:N:111:PRO:HD2	2.36	0.40
1:C:547:GLU:HG3	1:C:548:TYR:H	1.87	0.40
4:I:32:DC:H2"	4:I:33:DT:C5	2.56	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	
1	A	602/1040 (58%)	571 (95%)	31 (5%)	0	100	100
1	C	607/1040 (58%)	576 (95%)	31 (5%)	0	100	100
2	B	342/527 (65%)	329 (96%)	13 (4%)	0	100	100
2	D	342/527 (65%)	329 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	53/141 (38%)	52 (98%)	1 (2%)	0	100	100
7	N	32/141 (23%)	30 (94%)	2 (6%)	0	100	100
All	All	1978/3416 (58%)	1887 (95%)	91 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	509/933 (55%)	494 (97%)	15 (3%)	37	60
1	C	522/933 (56%)	507 (97%)	15 (3%)	37	60
2	B	292/469 (62%)	290 (99%)	2 (1%)	76	78
2	D	293/469 (62%)	289 (99%)	4 (1%)	59	71
7	H	9/122 (7%)	9 (100%)	0	100	100
7	N	17/122 (14%)	17 (100%)	0	100	100
All	All	1642/3048 (54%)	1606 (98%)	36 (2%)	45	65

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	476	LEU
1	A	496	ILE
1	A	563	LEU
1	A	588	ASN
1	A	607	GLU
1	A	638	VAL
1	A	655	LEU
1	A	658	MET
1	A	726	ILE
1	A	742	VAL
1	A	800	ASN
1	A	876	HIS

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Mol	Chain	Res	Type
1	A	920	LEU
1	A	983	GLU
1	A	1002	PHE
1	C	400	THR
1	C	476	LEU
1	C	541	LEU
1	C	587	LEU
1	C	631	ILE
1	C	655	LEU
1	C	657	LEU
1	C	658	MET
1	C	726	ILE
1	C	740	ASN
1	C	772	LEU
1	C	820	ASN
1	C	837	LEU
1	C	920	LEU
1	C	983	GLU
2	B	55	LEU
2	B	290	VAL
2	D	8	VAL
2	D	55	LEU
2	D	290	VAL
2	D	297	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	GLN
1	A	480	GLN
1	A	498	GLN
1	A	581	GLN
1	A	588	ASN
1	A	744	HIS
1	A	753	ASN
1	A	795	HIS
1	A	800	ASN
1	A	842	ASN
1	A	860	GLN
1	A	991	HIS
1	C	447	GLN
1	C	456	GLN

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Mol	Chain	Res	Type
1	C	463	GLN
1	C	482	HIS
1	C	495	GLN
1	C	515	HIS
1	C	525	ASN
1	C	636	GLN
1	C	637	ASN
1	C	740	ASN
1	C	750	HIS
1	C	753	ASN
1	C	912	ASN
1	C	937	HIS
2	B	4	GLN
2	B	16	GLN
2	B	27	GLN
2	B	53	ASN
2	B	94	HIS
2	B	101	ASN
2	B	181	HIS
2	B	201	GLN
2	B	213	ASN
2	B	222	HIS
2	B	282	GLN
2	D	4	GLN
2	D	16	GLN
2	D	23	ASN
2	D	53	ASN
2	D	94	HIS
2	D	100	ASN
2	D	201	GLN
2	D	213	ASN
2	D	282	GLN
7	N	117	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-20030. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

This section was not generated.

6.2 Central slices ⓘ

This section was not generated.

6.3 Largest variance slices ⓘ

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

This section was not generated.

6.5 Orthogonal surface views ⓘ

This section was not generated.

6.6 Mask visualisation ⓘ

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section was not generated.