



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:56 PM BST

PDB ID : 3JBW
EMDB ID: : EMD-6489
Title : Cryo-electron microscopy structure of RAG Paired Complex (with NBD, no symmetry)
Authors : Ru, H.; Chambers, M.G.; Fu, T.-M.; Tong, A.B.; Liao, M.; Wu, H.
Deposited on : 2015-10-21
Resolution : 4.63 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

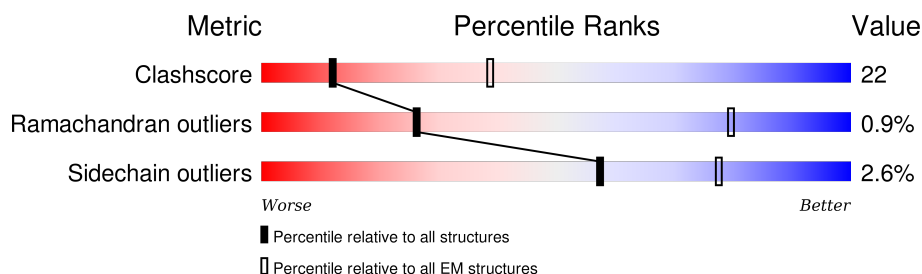
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.63 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.



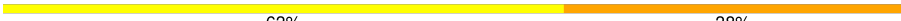
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	764	51% 29% • 19%
1	C	764	49% 31% •• 19%
2	B	533	37% 28% • 34%
2	D	533	39% 26% • 34%
3	E	34	15% 41% 44%
4	F	50	32% 50% 18%
5	G	61	15% 66% 20%
6	H	45	29% 42% 29%
7	I	16	13% 38% 50%

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Mol	Chain	Length	Quality of chain
7	J	16	 63% 38%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19997 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	622	Total	C	N	O	S	0	0
			5008	3134	901	936	37		
1	C	622	Total	C	N	O	S	0	0
			5008	3134	901	936	37		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	GLY	-	EXPRESSION TAG	UNP O13033
A	269	GLY	-	EXPRESSION TAG	UNP O13033
A	270	SER	-	EXPRESSION TAG	UNP O13033
C	268	GLY	-	EXPRESSION TAG	UNP O13033
C	269	GLY	-	EXPRESSION TAG	UNP O13033
C	270	SER	-	EXPRESSION TAG	UNP O13033

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	351	Total	C	N	O	S	0	0
			2714	1716	470	509	19		
2	D	351	Total	C	N	O	S	0	0
			2714	1716	470	509	19		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	EXPRESSION TAG	UNP Q1RLW7
B	-1	GLY	-	EXPRESSION TAG	UNP Q1RLW7
B	0	SER	-	EXPRESSION TAG	UNP Q1RLW7
D	-2	GLY	-	EXPRESSION TAG	UNP Q1RLW7
D	-1	GLY	-	EXPRESSION TAG	UNP Q1RLW7
D	0	SER	-	EXPRESSION TAG	UNP Q1RLW7

- Molecule 3 is a DNA chain called 12-RSS signal end forward strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	34	Total	C	N	O	P	0	0
			697	330	138	195	34		

- Molecule 4 is a DNA chain called Nicked 12-RSS intermediate reverse strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	50	Total	C	N	O	P	0	0
			1027	489	183	305	50		

- Molecule 5 is a DNA chain called Nicked 23-RSS intermediate reverse strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	61	Total	C	N	O	P	0	0
			1256	596	235	364	61		

- Molecule 6 is a DNA chain called Nicked 23-RSS intermediate forward strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	45	Total	C	N	O	P	0	0
			919	437	169	268	45		

- Molecule 7 is a DNA chain called 5'-D(P*GP*AP*TP*CP*TP*GP*GP*CP*CP*TP*GP*TP*CP*TP*TP*A)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	16	Total	C	N	O	P	0	0
			326	156	54	100	16		
7	J	16	Total	C	N	O	P	0	0
			326	156	54	100	16		

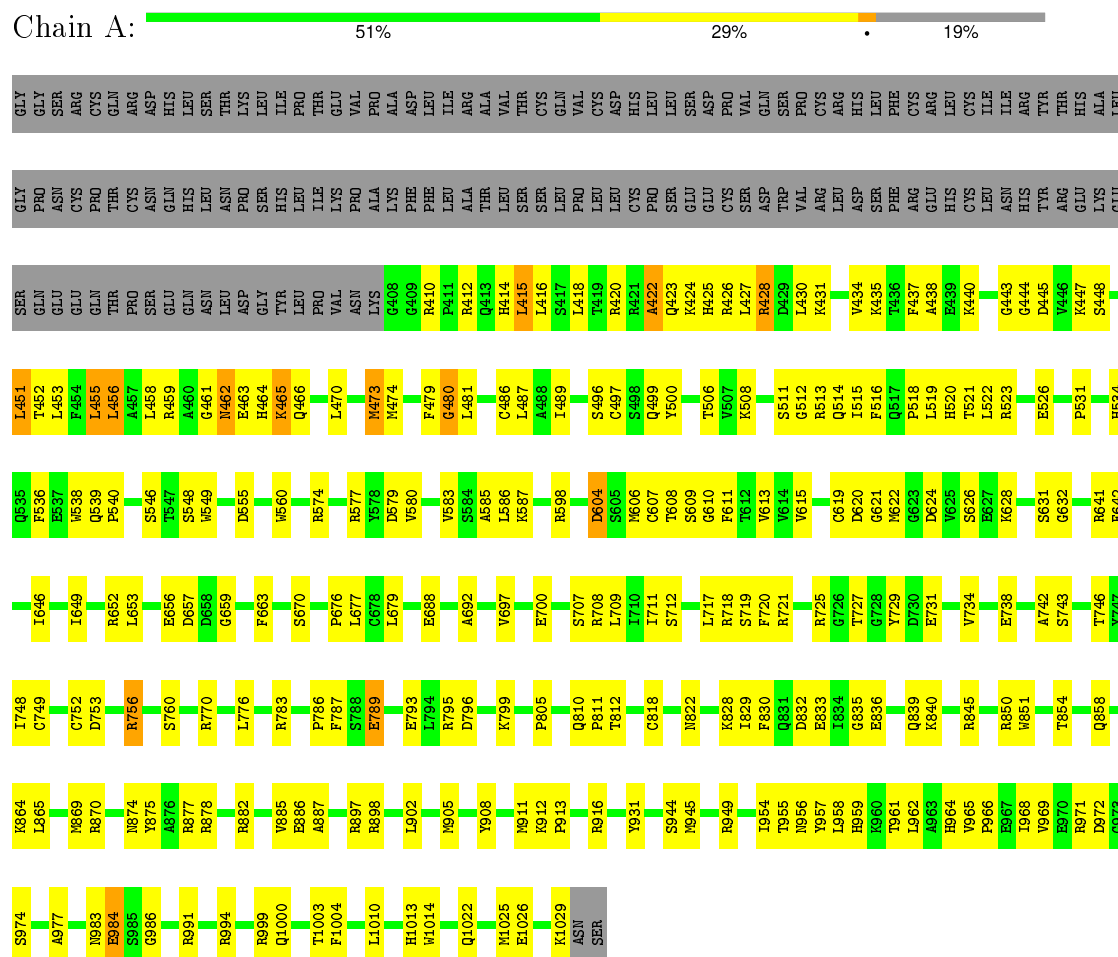
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

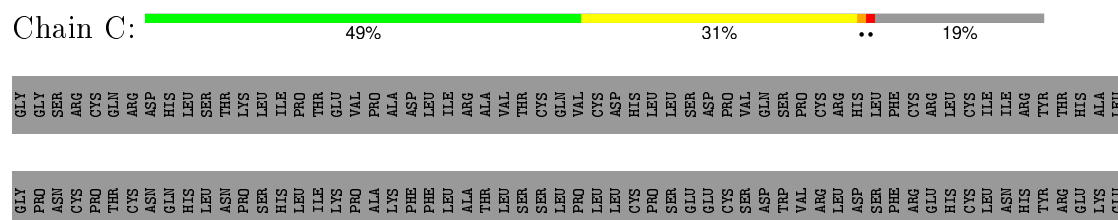
3 Residue-property plots

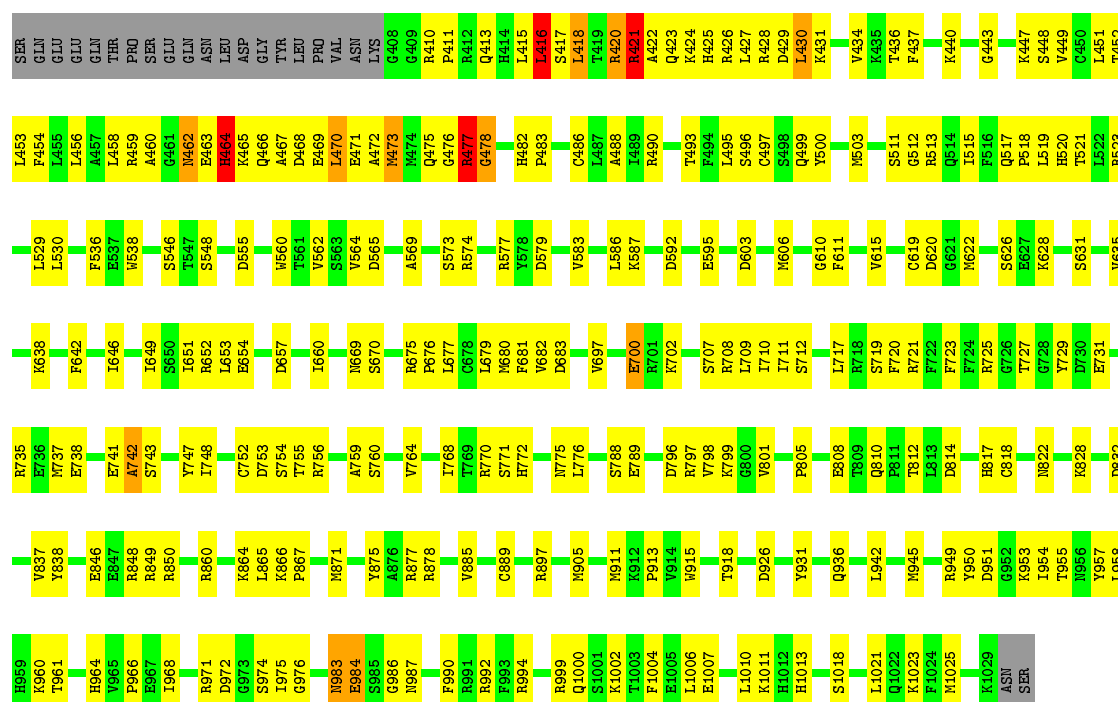
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: V(D)J recombination-activating protein 1

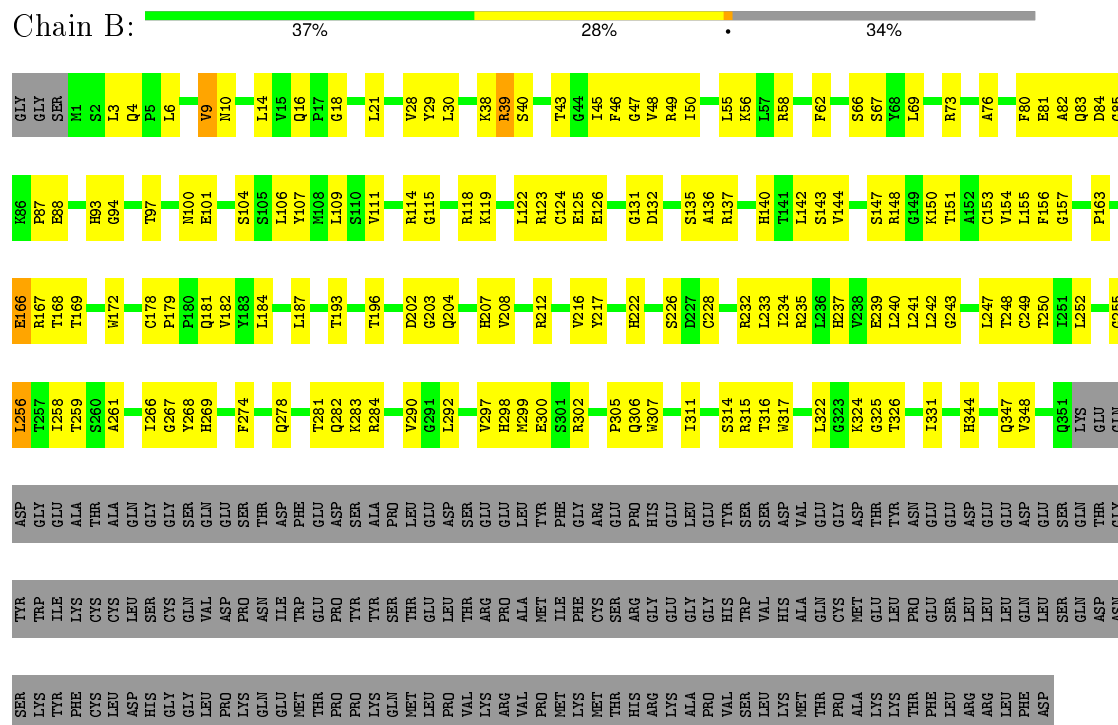


- Molecule 1: V(D)J recombination-activating protein 1

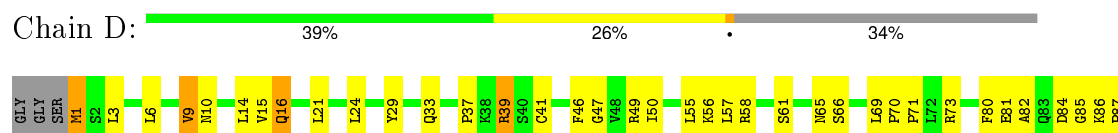


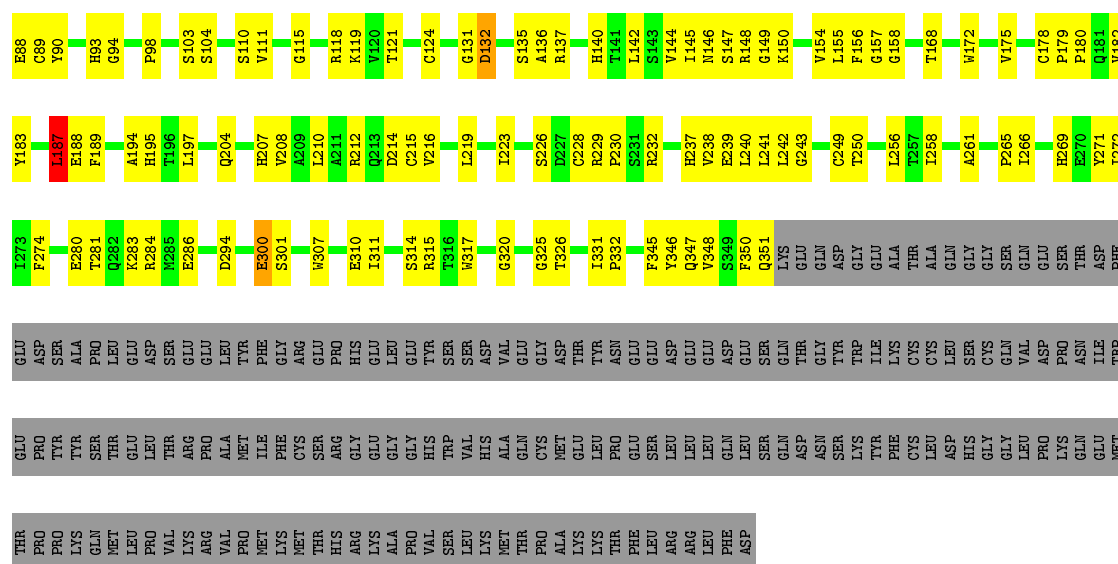


• Molecule 2: V(D)J recombination-activating protein 2



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





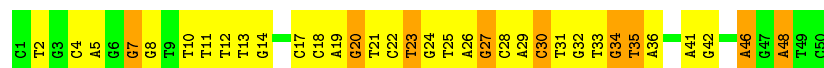
- Molecule 3: 12-RSS signal end forward strand

Chain E: 15% 41% 44%



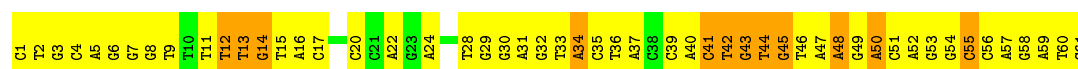
- Molecule 4: Nicked 12-RSS intermediate reverse strand

Chain F: 32% 50% 18%



- Molecule 5: Nicked 23-RSS intermediate reverse strand

Chain G: 15% 66% 20%



- Molecule 6: Nicked 23-RSS intermediate forward strand

Chain H: 29% 42% 29%

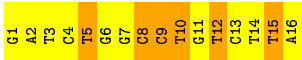


- Molecule 7: 5'-D(P*GP*AP*TP*CP*TP*GP*GP*CP*CP*TP*GP*TP*CP*TP*TP*A)-3',

Chain I: 13% 38% 50%



● Molecule 7: 5'-D(P*GP*AP*TP*CP*TP*GP*GP*CP*CP*TP*GP*TP*CP*TP*TP*A)-3',



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	14129	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 (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

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 >2	RMSZ	# Z >2
1	A	0.47	1/5106 (0.0%)	0.77	5/6867 (0.1%)
1	C	0.48	1/5106 (0.0%)	0.82	11/6867 (0.2%)
2	B	0.40	0/2784	0.66	1/3784 (0.0%)
2	D	0.41	0/2784	0.65	1/3784 (0.0%)
3	E	1.65	15/784 (1.9%)	1.33	11/1206 (0.9%)
4	F	1.42	8/1150 (0.7%)	1.32	7/1774 (0.4%)
5	G	1.74	24/1410 (1.7%)	1.41	23/2175 (1.1%)
6	H	2.29	44/1030 (4.3%)	1.65	26/1586 (1.6%)
7	I	2.15	13/363 (3.6%)	1.54	6/558 (1.1%)
7	J	1.57	6/363 (1.7%)	1.31	4/558 (0.7%)
All	All	0.98	112/20880 (0.5%)	0.98	95/29159 (0.3%)

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	2
All	All	0	3

The worst 5 of 112 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	42	DT	P-O5'	-19.75	1.40	1.59
6	H	2	DA	C3'-O3'	19.18	1.68	1.44
5	G	45	DG	C3'-O3'	17.23	1.66	1.44
6	H	5	DG	C3'-O3'	17.20	1.66	1.44
6	H	3	DC	N3-C4	15.62	1.44	1.33

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	6	DT	O5'-P-OP2	22.18	137.32	110.70
6	H	3	DC	OP1-P-OP2	-14.91	97.24	119.60
6	H	3	DC	O4'-C1'-N1	12.66	116.86	108.00
5	G	41	DC	OP2-P-O3'	11.06	129.54	105.20
5	G	42	DT	O5'-P-OP1	-10.51	96.25	105.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	462	ASN	Peptide
1	C	477	ARG	Peptide
1	C	742	ALA	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	A	5008	0	4968	224	0
1	C	5008	0	4968	233	0
2	B	2714	0	2665	124	0
2	D	2714	0	2665	115	0
3	E	697	0	379	36	0
4	F	1027	0	566	57	0
5	G	1256	0	686	82	0
6	H	919	0	506	60	0
7	I	326	0	183	32	0
7	J	326	0	183	36	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
All	All	19997	0	17769	828	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 22.

The worst 5 of 828 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)
6:H:5:DG:O3'	6:H:5:DG:C3'	1.66	1.44
5:G:45:DG:O3'	5:G:45:DG:C3'	1.66	1.44
6:H:2:DA:O3'	6:H:2:DA:C3'	1.68	1.38
2:D:58:ARG:HH12	7:I:6:DG:H5''	1.20	1.02
5:G:12:DT:H2''	5:G:13:DT:H5'	1.41	1.01

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	620/764 (81%)	574 (93%)	38 (6%)	8 (1%)	15	60
1	C	620/764 (81%)	572 (92%)	42 (7%)	6 (1%)	19	65
2	B	349/533 (66%)	332 (95%)	15 (4%)	2 (1%)	30	74
2	D	349/533 (66%)	335 (96%)	13 (4%)	1 (0%)	46	83
All	All	1938/2594 (75%)	1813 (94%)	108 (6%)	17 (1%)	26	67

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	LYS
1	A	465	LYS
1	A	473	MET
1	C	416	LEU
1	C	464	HIS

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	548/681 (80%)	538 (98%)	10 (2%)	66	87
1	C	548/681 (80%)	528 (96%)	20 (4%)	42	75
2	B	303/465 (65%)	296 (98%)	7 (2%)	58	83
2	D	303/465 (65%)	295 (97%)	8 (3%)	54	81
All	All	1702/2292 (74%)	1657 (97%)	45 (3%)	57	81

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	448	SER
1	C	565	ASP
2	D	175	VAL
1	C	470	LEU
1	C	586	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	100	ASN
2	B	278	GLN
1	C	466	GLN
1	A	983	ASN
1	C	462	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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.