



# wwPDB EM Model Validation Summary Report ⓘ

May 21, 2020 – 07:53 AM EDT

PDB ID : 6LXW  
EMDB ID : EMD-30008  
Title : Cryo-EM structure of human secretory immunoglobulin A in complex with the N-terminal domain of SpsA  
Authors : Wang, Y.; Wang, G.; Li, Y.; Xiao, J.  
Deposited on : 2020-02-12  
Resolution : 3.27 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.10.1

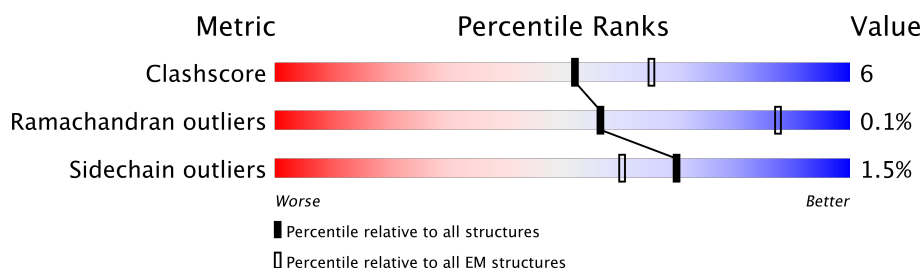
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.27 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	291	63% 14% 23%
1	B	291	60% 15% 25%
1	C	291	63% 12% • 24%
1	D	291	67% 11% • 21%
2	J	167	68% 8% • 23%
3	P	573	72% 16% • 10%
4	S	317	17% • 81%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12299 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 Interleukin-2,Immunoglobulin heavy constant alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	225	Total	C	N	O	S	0	0
			1707	1076	291	330	10		
1	B	218	Total	C	N	O	S	0	0
			1660	1048	286	317	9		
1	C	221	Total	C	N	O	S	0	0
			1682	1062	290	321	9		
1	D	229	Total	C	N	O	S	0	0
			1740	1097	298	335	10		

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	ARG	-	linker	UNP P60568
A	204	ILE	-	linker	UNP P60568
A	205	HIS	-	linker	UNP P60568
A	206	MET	-	linker	UNP P60568
A	207	SER	-	linker	UNP P60568
A	208	ALA	-	linker	UNP P60568
A	209	TRP	-	linker	UNP P60568
A	210	SER	-	linker	UNP P60568
A	211	HIS	-	linker	UNP P60568
A	212	PRO	-	linker	UNP P60568
A	213	GLN	-	linker	UNP P60568
A	214	PHE	-	linker	UNP P60568
A	215	GLU	-	linker	UNP P60568
A	216	LYS	-	linker	UNP P60568
A	217	GLY	-	linker	UNP P60568
A	218	GLY	-	linker	UNP P60568
A	219	GLY	-	linker	UNP P60568
A	220	SER	-	linker	UNP P60568
A	221	GLY	-	linker	UNP P60568
A	222	GLY	-	linker	UNP P60568
A	223	GLY	-	linker	UNP P60568
A	224	SER	-	linker	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
A	225	GLY	-	linker	UNP P60568
A	226	GLY	-	linker	UNP P60568
A	227	SER	-	linker	UNP P60568
A	228	ALA	-	linker	UNP P60568
A	229	TRP	-	linker	UNP P60568
A	230	SER	-	linker	UNP P60568
A	231	HIS	-	linker	UNP P60568
A	232	PRO	-	linker	UNP P60568
A	233	GLN	-	linker	UNP P60568
A	234	PHE	-	linker	UNP P60568
A	235	GLU	-	linker	UNP P60568
A	236	LYS	-	linker	UNP P60568
A	237	ILE	-	linker	UNP P60568
A	238	ASP	-	linker	UNP P60568
A	239	THR	-	linker	UNP P60568
A	240	THR	-	linker	UNP P60568
B	203	ARG	-	linker	UNP P60568
B	204	ILE	-	linker	UNP P60568
B	205	HIS	-	linker	UNP P60568
B	206	MET	-	linker	UNP P60568
B	207	SER	-	linker	UNP P60568
B	208	ALA	-	linker	UNP P60568
B	209	TRP	-	linker	UNP P60568
B	210	SER	-	linker	UNP P60568
B	211	HIS	-	linker	UNP P60568
B	212	PRO	-	linker	UNP P60568
B	213	GLN	-	linker	UNP P60568
B	214	PHE	-	linker	UNP P60568
B	215	GLU	-	linker	UNP P60568
B	216	LYS	-	linker	UNP P60568
B	217	GLY	-	linker	UNP P60568
B	218	GLY	-	linker	UNP P60568
B	219	GLY	-	linker	UNP P60568
B	220	SER	-	linker	UNP P60568
B	221	GLY	-	linker	UNP P60568
B	222	GLY	-	linker	UNP P60568
B	223	GLY	-	linker	UNP P60568
B	224	SER	-	linker	UNP P60568
B	225	GLY	-	linker	UNP P60568
B	226	GLY	-	linker	UNP P60568
B	227	SER	-	linker	UNP P60568
B	228	ALA	-	linker	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
B	229	TRP	-	linker	UNP P60568
B	230	SER	-	linker	UNP P60568
B	231	HIS	-	linker	UNP P60568
B	232	PRO	-	linker	UNP P60568
B	233	GLN	-	linker	UNP P60568
B	234	PHE	-	linker	UNP P60568
B	235	GLU	-	linker	UNP P60568
B	236	LYS	-	linker	UNP P60568
B	237	ILE	-	linker	UNP P60568
B	238	ASP	-	linker	UNP P60568
B	239	THR	-	linker	UNP P60568
B	240	THR	-	linker	UNP P60568
C	203	ARG	-	linker	UNP P60568
C	204	ILE	-	linker	UNP P60568
C	205	HIS	-	linker	UNP P60568
C	206	MET	-	linker	UNP P60568
C	207	SER	-	linker	UNP P60568
C	208	ALA	-	linker	UNP P60568
C	209	TRP	-	linker	UNP P60568
C	210	SER	-	linker	UNP P60568
C	211	HIS	-	linker	UNP P60568
C	212	PRO	-	linker	UNP P60568
C	213	GLN	-	linker	UNP P60568
C	214	PHE	-	linker	UNP P60568
C	215	GLU	-	linker	UNP P60568
C	216	LYS	-	linker	UNP P60568
C	217	GLY	-	linker	UNP P60568
C	218	GLY	-	linker	UNP P60568
C	219	GLY	-	linker	UNP P60568
C	220	SER	-	linker	UNP P60568
C	221	GLY	-	linker	UNP P60568
C	222	GLY	-	linker	UNP P60568
C	223	GLY	-	linker	UNP P60568
C	224	SER	-	linker	UNP P60568
C	225	GLY	-	linker	UNP P60568
C	226	GLY	-	linker	UNP P60568
C	227	SER	-	linker	UNP P60568
C	228	ALA	-	linker	UNP P60568
C	229	TRP	-	linker	UNP P60568
C	230	SER	-	linker	UNP P60568
C	231	HIS	-	linker	UNP P60568
C	232	PRO	-	linker	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
C	233	GLN	-	linker	UNP P60568
C	234	PHE	-	linker	UNP P60568
C	235	GLU	-	linker	UNP P60568
C	236	LYS	-	linker	UNP P60568
C	237	ILE	-	linker	UNP P60568
C	238	ASP	-	linker	UNP P60568
C	239	THR	-	linker	UNP P60568
C	240	THR	-	linker	UNP P60568
D	203	ARG	-	linker	UNP P60568
D	204	ILE	-	linker	UNP P60568
D	205	HIS	-	linker	UNP P60568
D	206	MET	-	linker	UNP P60568
D	207	SER	-	linker	UNP P60568
D	208	ALA	-	linker	UNP P60568
D	209	TRP	-	linker	UNP P60568
D	210	SER	-	linker	UNP P60568
D	211	HIS	-	linker	UNP P60568
D	212	PRO	-	linker	UNP P60568
D	213	GLN	-	linker	UNP P60568
D	214	PHE	-	linker	UNP P60568
D	215	GLU	-	linker	UNP P60568
D	216	LYS	-	linker	UNP P60568
D	217	GLY	-	linker	UNP P60568
D	218	GLY	-	linker	UNP P60568
D	219	GLY	-	linker	UNP P60568
D	220	SER	-	linker	UNP P60568
D	221	GLY	-	linker	UNP P60568
D	222	GLY	-	linker	UNP P60568
D	223	GLY	-	linker	UNP P60568
D	224	SER	-	linker	UNP P60568
D	225	GLY	-	linker	UNP P60568
D	226	GLY	-	linker	UNP P60568
D	227	SER	-	linker	UNP P60568
D	228	ALA	-	linker	UNP P60568
D	229	TRP	-	linker	UNP P60568
D	230	SER	-	linker	UNP P60568
D	231	HIS	-	linker	UNP P60568
D	232	PRO	-	linker	UNP P60568
D	233	GLN	-	linker	UNP P60568
D	234	PHE	-	linker	UNP P60568
D	235	GLU	-	linker	UNP P60568
D	236	LYS	-	linker	UNP P60568

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Chain	Residue	Modelled	Actual	Comment	Reference
D	237	ILE	-	linker	UNP P60568
D	238	ASP	-	linker	UNP P60568
D	239	THR	-	linker	UNP P60568
D	240	THR	-	linker	UNP P60568

- Molecule 2 is a protein called Immunoglobulin J chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	128	Total	C	N	O	S	0	0
			1016	626	177	204	9		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	137	HIS	-	expression tag	UNP P01591
J	138	HIS	-	expression tag	UNP P01591
J	139	HIS	-	expression tag	UNP P01591
J	140	HIS	-	expression tag	UNP P01591
J	141	HIS	-	expression tag	UNP P01591
J	142	HIS	-	expression tag	UNP P01591
J	143	HIS	-	expression tag	UNP P01591
J	144	HIS	-	expression tag	UNP P01591

- Molecule 3 is a protein called Polymeric immunoglobulin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	513	Total	C	N	O	S	0	0
			3988	2519	693	756	20		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	548	HIS	-	expression tag	UNP P01833
P	549	HIS	-	expression tag	UNP P01833
P	550	HIS	-	expression tag	UNP P01833
P	551	HIS	-	expression tag	UNP P01833
P	552	HIS	-	expression tag	UNP P01833
P	553	HIS	-	expression tag	UNP P01833
P	554	HIS	-	expression tag	UNP P01833
P	555	HIS	-	expression tag	UNP P01833

- Molecule 4 is a protein called SigA binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	S	61	Total	C	N	O	0	0
			506	312	83	111		

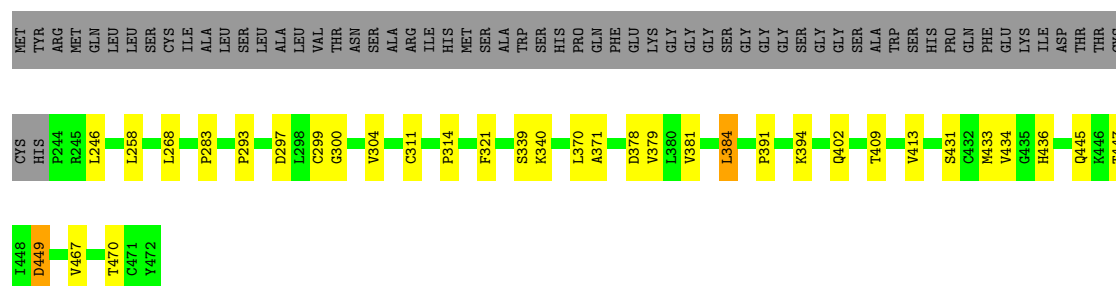
There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	8	MET	-	initiating methionine	UNP O33753
S	9	GLY	-	expression tag	UNP O33753
S	10	SER	-	expression tag	UNP O33753
S	11	HIS	-	expression tag	UNP O33753
S	12	HIS	-	expression tag	UNP O33753
S	13	HIS	-	expression tag	UNP O33753
S	14	HIS	-	expression tag	UNP O33753
S	15	HIS	-	expression tag	UNP O33753
S	16	HIS	-	expression tag	UNP O33753
S	17	HIS	-	expression tag	UNP O33753
S	18	HIS	-	expression tag	UNP O33753
S	19	GLY	-	expression tag	UNP O33753
S	20	SER	-	expression tag	UNP O33753
S	21	ASP	-	expression tag	UNP O33753
S	22	TYR	-	expression tag	UNP O33753
S	23	ASP	-	expression tag	UNP O33753
S	24	ILE	-	expression tag	UNP O33753
S	25	PRO	-	expression tag	UNP O33753
S	26	THR	-	expression tag	UNP O33753
S	27	THR	-	expression tag	UNP O33753
S	28	GLU	-	expression tag	UNP O33753
S	29	ASN	-	expression tag	UNP O33753
S	30	LEU	-	expression tag	UNP O33753
S	31	TYR	-	expression tag	UNP O33753
S	32	PHE	-	expression tag	UNP O33753
S	33	GLN	-	expression tag	UNP O33753
S	34	GLY	-	expression tag	UNP O33753
S	35	SER	-	expression tag	UNP O33753
S	36	GLU	-	expression tag	UNP O33753
S	37	PHE	-	expression tag	UNP O33753



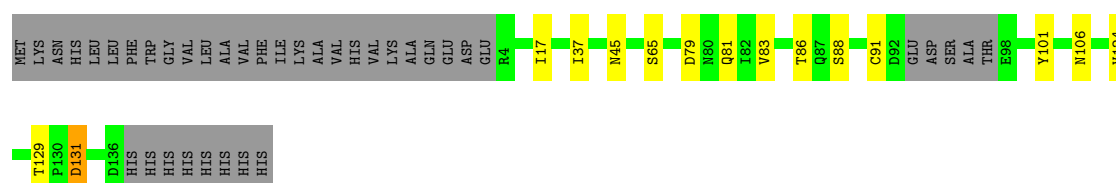


Chain D:  67% 11% 21%



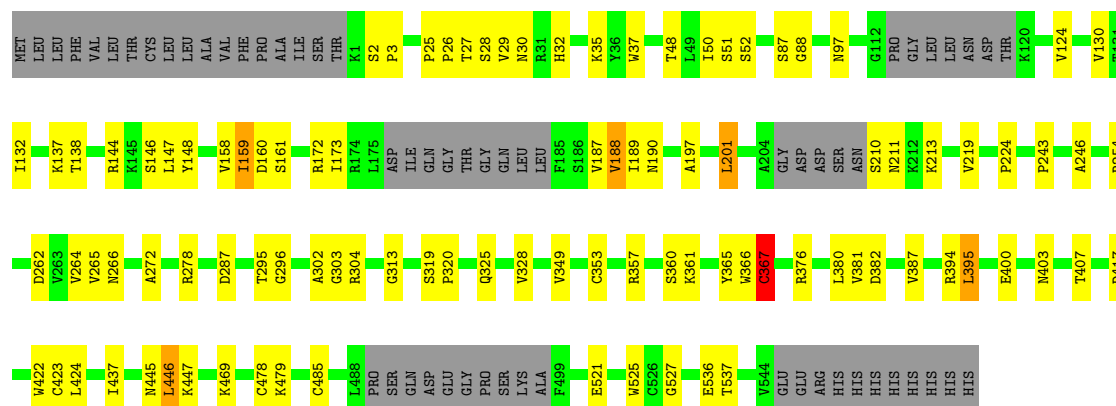
- Molecule 2: Immunoglobulin J chain

Chain J:  68% 8% 23%



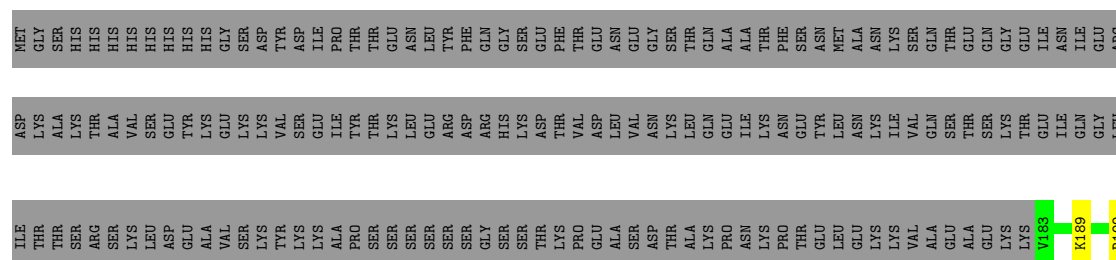
- Molecule 3: Polymeric immunoglobulin receptor

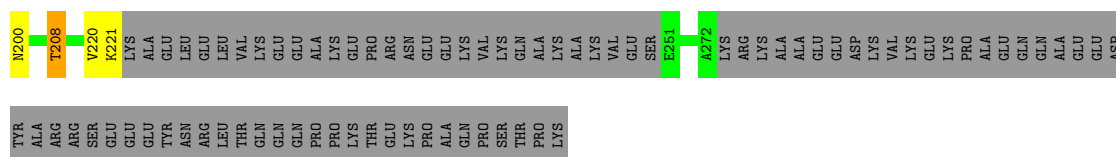
Chain P:  72% 16% • 10%



- Molecule 4: SigA binding protein

Chain S:  17% . 81%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	280791	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 ( $e^-/\text{\AA}^2$ )	59.74	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (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	A	0.67	0/1747	0.72	1/2384 (0.0%)
1	B	0.58	0/1700	0.69	0/2320
1	C	0.54	1/1724 (0.1%)	0.67	1/2354 (0.0%)
1	D	0.64	0/1783	0.70	1/2435 (0.0%)
2	J	0.66	0/1030	0.72	1/1401 (0.1%)
3	P	0.77	2/4073 (0.0%)	0.71	4/5526 (0.1%)
4	S	0.54	0/508	0.59	0/676
All	All	0.67	3/12565 (0.0%)	0.70	8/17096 (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
1	A	0	1
2	J	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	367	CYS	CB-SG	-6.35	1.71	1.82
3	P	265	VAL	CB-CG2	-6.15	1.40	1.52
1	C	402	GLN	C-N	-5.80	1.20	1.34

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	131	ASP	CB-CG-OD1	8.56	126.00	118.30
3	P	446	LEU	CA-CB-CG	6.71	130.72	115.30
1	C	271	LEU	CA-CB-CG	6.65	130.60	115.30
3	P	201	LEU	CA-CB-CG	6.38	129.97	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	384	LEU	CB-CG-CD2	-5.68	101.33	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	ASP	Peptide
2	J	79	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	A	1707	0	1688	25	0
1	B	1660	0	1650	27	0
1	C	1682	0	1676	22	0
1	D	1740	0	1722	17	0
2	J	1016	0	999	8	0
3	P	3988	0	3905	59	0
4	S	506	0	504	5	0
All	All	12299	0	12144	151	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 6.

The worst 5 of 151 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:263:ASN:HA	1:C:308:LEU:O	1.74	0.88
1:B:383:TRP:HE1	1:B:415:SER:HG	1.30	0.80
1:B:277:VAL:HG11	1:B:304:VAL:HG21	1.77	0.67
3:P:224:PRO:HG3	3:P:304:ARG:HH22	1.62	0.63
1:B:324:THR:HG23	1:B:335:THR:HG22	1.80	0.63

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	221/291 (76%)	184 (83%)	37 (17%)	0	100	100
1	B	214/291 (74%)	183 (86%)	31 (14%)	0	100	100
1	C	219/291 (75%)	190 (87%)	29 (13%)	0	100	100
1	D	227/291 (78%)	196 (86%)	31 (14%)	0	100	100
2	J	124/167 (74%)	102 (82%)	22 (18%)	0	100	100
3	P	503/573 (88%)	449 (89%)	53 (10%)	1 (0%)	49	79
4	S	57/317 (18%)	53 (93%)	3 (5%)	1 (2%)	9	39
All	All	1565/2221 (70%)	1357 (87%)	206 (13%)	2 (0%)	56	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	S	208	THR
3	P	161	SER

### 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	191/244 (78%)	188 (98%)	3 (2%)	65	83
1	B	186/244 (76%)	186 (100%)	0	100	100
1	C	189/244 (78%)	186 (98%)	3 (2%)	65	83
1	D	195/244 (80%)	190 (97%)	5 (3%)	49	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	121/155 (78%)	118 (98%)	3 (2%)	50	76
3	P	438/490 (89%)	432 (99%)	6 (1%)	69	84
4	S	55/283 (19%)	55 (100%)	0	100	100
All	All	1375/1904 (72%)	1355 (98%)	20 (2%)	70	84

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	467	VAL
1	D	470	THR
3	P	188	VAL
1	D	447	THR
1	D	449	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	89	ASN
3	P	30	ASN
3	P	481	ASN
2	J	81	GLN
3	P	111	GLN

### 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 [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.