



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:53 PM UTC

PDB ID : 9QSM / pdb\_00009qsm  
Title : small molecule inhibitor in complex with PD-L1  
Authors : Muszak, D.; Kocik-Krol, J.; Zaber, J.; Kruc, O.; Palej, U.; Fijolkowska, K.; Maslanka, A.; Magiera-Mularz, K.; Plewka, J.; Stec, M.; Siedlar, M.; Musielak, B.; Kitel, R.; Skalniak, L.; Surmiak, E.  
Deposited on : 2025-04-05  
Resolution : 1.75 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](mailto: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:

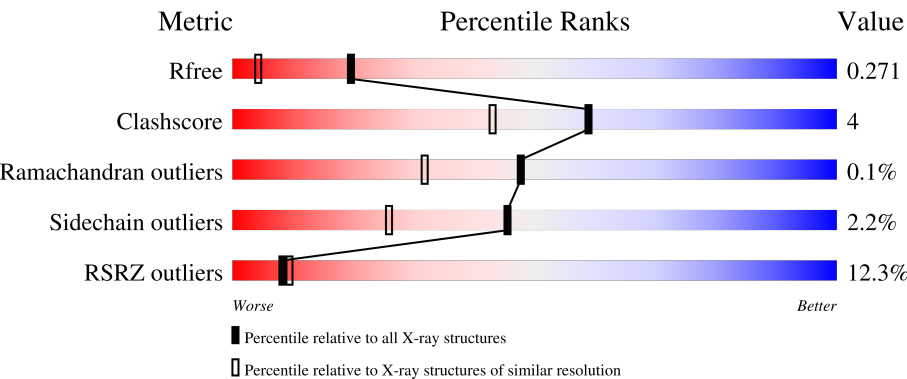
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	128	<div><div>17%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>81%9%•9%</div></div>
1	B	128	<div><div>5%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>82%8%••9%</div></div>
1	C	128	<div><div>9%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>77%11%••9%</div></div>
1	D	128	<div><div>12%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>78%13%9%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	128	<div> <div>8%</div> <div>79%</div> <div>9%</div> <div>••</div> <div>9%</div> </div>
1	F	128	<div> <div>15%</div> <div>82%</div> <div>9%</div> <div>•</div> <div>8%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5806 atoms, of which 0 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 Programmed cell death 1 ligand 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	0	0	0
			914	585	152	172	5			
1	B	117	Total	C	N	O	S	0	0	0
			929	593	156	175	5			
1	C	117	Total	C	N	O	S	0	0	0
			933	596	157	175	5			
1	D	117	Total	C	N	O	S	0	0	0
			929	593	156	175	5			
1	E	117	Total	C	N	O	S	0	0	0
			936	599	156	176	5			
1	F	118	Total	C	N	O	S	0	0	0
			933	597	155	176	5			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	ALA	-	expression tag	UNP Q9NZQ7
A	122	ALA	-	expression tag	UNP Q9NZQ7
A	123	ALA	-	expression tag	UNP Q9NZQ7
A	124	LEU	-	expression tag	UNP Q9NZQ7
A	125	GLU	-	expression tag	UNP Q9NZQ7
A	126	HIS	-	expression tag	UNP Q9NZQ7
A	127	HIS	-	expression tag	UNP Q9NZQ7
A	128	HIS	-	expression tag	UNP Q9NZQ7
A	129	HIS	-	expression tag	UNP Q9NZQ7
A	130	HIS	-	expression tag	UNP Q9NZQ7
A	131	HIS	-	expression tag	UNP Q9NZQ7
B	121	ALA	-	expression tag	UNP Q9NZQ7
B	122	ALA	-	expression tag	UNP Q9NZQ7
B	123	ALA	-	expression tag	UNP Q9NZQ7
B	124	LEU	-	expression tag	UNP Q9NZQ7
B	125	GLU	-	expression tag	UNP Q9NZQ7
B	126	HIS	-	expression tag	UNP Q9NZQ7

*Continued on next page...*

*Continued from previous page...*

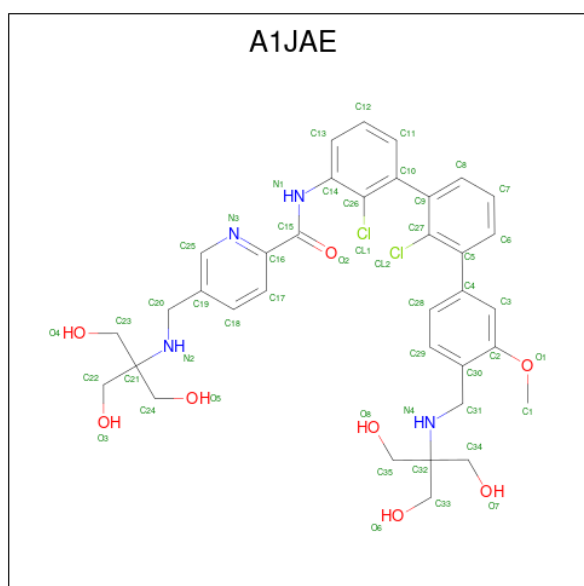
Chain	Residue	Modelled	Actual	Comment	Reference
B	127	HIS	-	expression tag	UNP Q9NZQ7
B	128	HIS	-	expression tag	UNP Q9NZQ7
B	129	HIS	-	expression tag	UNP Q9NZQ7
B	130	HIS	-	expression tag	UNP Q9NZQ7
B	131	HIS	-	expression tag	UNP Q9NZQ7
C	121	ALA	-	expression tag	UNP Q9NZQ7
C	122	ALA	-	expression tag	UNP Q9NZQ7
C	123	ALA	-	expression tag	UNP Q9NZQ7
C	124	LEU	-	expression tag	UNP Q9NZQ7
C	125	GLU	-	expression tag	UNP Q9NZQ7
C	126	HIS	-	expression tag	UNP Q9NZQ7
C	127	HIS	-	expression tag	UNP Q9NZQ7
C	128	HIS	-	expression tag	UNP Q9NZQ7
C	129	HIS	-	expression tag	UNP Q9NZQ7
C	130	HIS	-	expression tag	UNP Q9NZQ7
C	131	HIS	-	expression tag	UNP Q9NZQ7
D	121	ALA	-	expression tag	UNP Q9NZQ7
D	122	ALA	-	expression tag	UNP Q9NZQ7
D	123	ALA	-	expression tag	UNP Q9NZQ7
D	124	LEU	-	expression tag	UNP Q9NZQ7
D	125	GLU	-	expression tag	UNP Q9NZQ7
D	126	HIS	-	expression tag	UNP Q9NZQ7
D	127	HIS	-	expression tag	UNP Q9NZQ7
D	128	HIS	-	expression tag	UNP Q9NZQ7
D	129	HIS	-	expression tag	UNP Q9NZQ7
D	130	HIS	-	expression tag	UNP Q9NZQ7
D	131	HIS	-	expression tag	UNP Q9NZQ7
E	121	ALA	-	expression tag	UNP Q9NZQ7
E	122	ALA	-	expression tag	UNP Q9NZQ7
E	123	ALA	-	expression tag	UNP Q9NZQ7
E	124	LEU	-	expression tag	UNP Q9NZQ7
E	125	GLU	-	expression tag	UNP Q9NZQ7
E	126	HIS	-	expression tag	UNP Q9NZQ7
E	127	HIS	-	expression tag	UNP Q9NZQ7
E	128	HIS	-	expression tag	UNP Q9NZQ7
E	129	HIS	-	expression tag	UNP Q9NZQ7
E	130	HIS	-	expression tag	UNP Q9NZQ7
E	131	HIS	-	expression tag	UNP Q9NZQ7
F	121	ALA	-	expression tag	UNP Q9NZQ7
F	122	ALA	-	expression tag	UNP Q9NZQ7
F	123	ALA	-	expression tag	UNP Q9NZQ7
F	124	LEU	-	expression tag	UNP Q9NZQ7

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	125	GLU	-	expression tag	UNP Q9NZQ7
F	126	HIS	-	expression tag	UNP Q9NZQ7
F	127	HIS	-	expression tag	UNP Q9NZQ7
F	128	HIS	-	expression tag	UNP Q9NZQ7
F	129	HIS	-	expression tag	UNP Q9NZQ7
F	130	HIS	-	expression tag	UNP Q9NZQ7
F	131	HIS	-	expression tag	UNP Q9NZQ7

- Molecule 2 is {N}-[2-chloranyl-3-[2-chloranyl-3-[4-[[[2-(hydroxymethyl)-1,3-bis(oxidanyl)propan-2-yl]amino]methyl]-3-methoxy-phenyl]phenyl]phenyl]-5-[[[2-(hydroxymethyl)-1,3-bis(oxidanyl)propan-2-yl]amino]methyl]pyridine-2-carboxamide (CCD ID: A1JAE) (formula:  $C_{35}H_{40}Cl_2N_4O_8$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	O	0	0
			49	35	2	4	8		
2	D	1	Total	C	Cl	N	O	0	0
			49	35	2	4	8		
2	E	1	Total	C	Cl	N	O	0	0
			49	35	2	4	8		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		

Continued on next page...

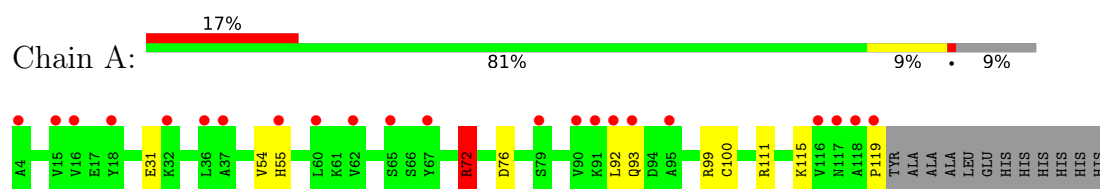
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	14	Total 14	O 14	0	0
3	C	16	Total 16	O 16	0	0
3	D	16	Total 16	O 16	0	0
3	E	21	Total 21	O 21	0	0
3	F	8	Total 8	O 8	0	0

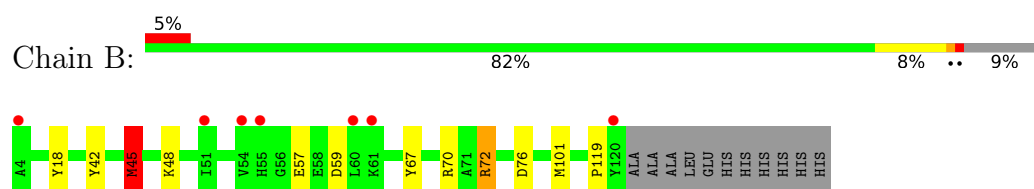
### 3 Residue-property plots

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 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.

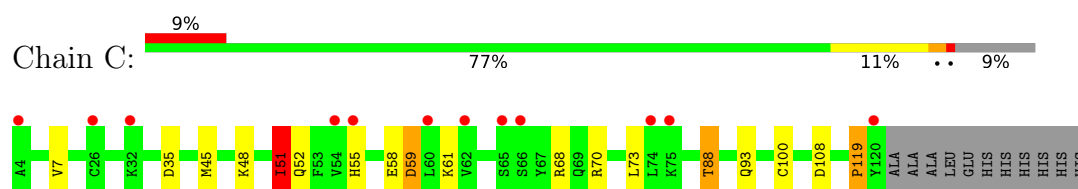
- Molecule 1: Programmed cell death 1 ligand 1



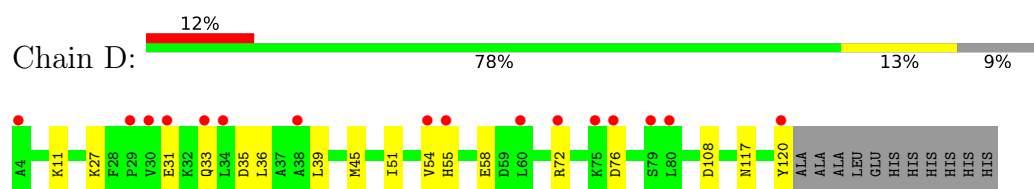
- Molecule 1: Programmed cell death 1 ligand 1



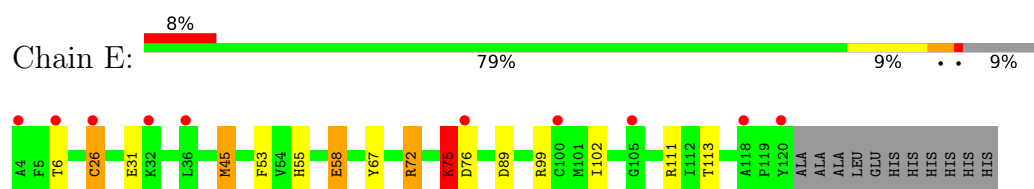
- Molecule 1: Programmed cell death 1 ligand 1



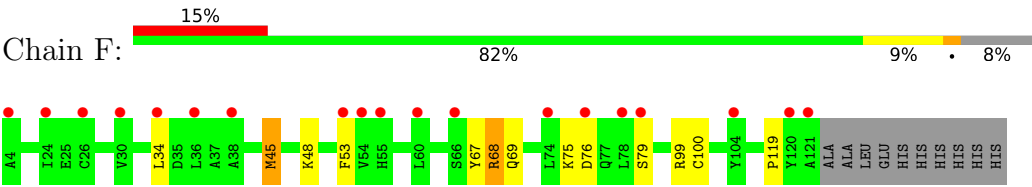
- Molecule 1: Programmed cell death 1 ligand 1



- Molecule 1: Programmed cell death 1 ligand 1



- Molecule 1: Programmed cell death 1 ligand 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.52Å 75.00Å 74.61Å 90.00° 95.49° 90.00°	Depositor
Resolution (Å)	47.62 – 1.75 47.62 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.62-1.75) 98.8 (47.62-1.75)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, $R_{free}$	0.244 , 0.270 0.244 , 0.271	Depositor DCC
$R_{free}$ test set	3656 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 18.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5806	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0877e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1JAE

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	0.64	0/930	1.49	8/1260 (0.6%)
1	B	0.67	0/945	1.33	7/1279 (0.5%)
1	C	0.67	0/949	1.46	11/1283 (0.9%)
1	D	0.66	0/945	1.36	6/1279 (0.5%)
1	E	0.68	0/953	1.42	11/1290 (0.9%)
1	F	0.63	0/950	1.28	3/1288 (0.2%)
All	All	0.66	0/5672	1.39	46/7679 (0.6%)

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	3
1	B	0	1
1	D	0	1
1	E	0	2
1	F	0	1
All	All	0	8

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ARG	CD-NE-CZ	16.66	147.72	124.40
1	A	55	HIS	CA-CB-CG	10.71	124.52	113.80
1	E	72	ARG	CD-NE-CZ	10.71	139.39	124.40
1	C	88	THR	OG1-CB-CG2	-10.56	88.17	109.30
1	A	72	ARG	NE-CZ-NH2	-8.94	111.16	119.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	6	THR	CA-CB-OG1	-8.61	96.68	109.60
1	C	55	HIS	CA-CB-CG	8.46	122.26	113.80
1	E	26	CYS	CB-CA-C	8.09	124.34	109.70
1	B	72	ARG	CD-NE-CZ	8.05	135.66	124.40
1	F	119	PRO	CB-CA-C	7.90	121.68	111.64
1	E	72	ARG	NE-CZ-NH2	-7.65	112.32	119.20
1	A	72	ARG	NE-CZ-NH1	7.54	129.03	121.50
1	B	45	MET	CG-SD-CE	7.21	116.75	100.90
1	A	93	GLN	N-CA-CB	-7.17	97.83	110.39
1	E	72	ARG	CB-CG-CD	6.74	126.79	111.30
1	D	76	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	31	GLU	CB-CA-C	6.38	122.17	110.11
1	F	76	ASP	CA-CB-CG	6.38	118.98	112.60
1	C	58	GLU	CB-CA-C	6.36	120.53	109.65
1	A	76	ASP	CA-CB-CG	6.34	118.94	112.60
1	D	58	GLU	CB-CA-C	6.32	120.45	109.65
1	C	48	LYS	CG-CD-CE	6.26	125.71	111.30
1	A	72	ARG	CB-CG-CD	6.16	125.46	111.30
1	E	76	ASP	CA-CB-CG	6.09	118.69	112.60
1	B	72	ARG	NE-CZ-NH2	-6.07	113.74	119.20
1	B	76	ASP	CA-CB-CG	5.84	118.44	112.60
1	C	45	MET	CG-SD-CE	-5.72	88.31	100.90
1	D	27	LYS	CB-CG-CD	5.63	124.25	111.30
1	D	11	LYS	CB-CA-C	-5.59	100.88	110.16
1	C	52	GLN	N-CA-CB	-5.56	101.47	110.81
1	C	35	ASP	CA-CB-CG	5.56	118.16	112.60
1	E	75	LYS	CB-CG-CD	5.55	124.06	111.30
1	E	72	ARG	NE-CZ-NH1	5.52	127.02	121.50
1	C	51	ILE	CA-CB-CG1	5.51	119.77	110.40
1	C	59	ASP	CA-CB-CG	5.42	118.03	112.60
1	F	68	ARG	CB-CA-C	5.40	117.94	110.16
1	B	70	ARG	CD-NE-CZ	5.38	131.93	124.40
1	E	58	GLU	CG-CD-OE1	-5.31	106.19	118.40
1	C	68	ARG	CB-CA-C	5.27	117.39	110.06
1	C	70	ARG	CD-NE-CZ	5.19	131.66	124.40
1	D	120	TYR	CA-C-O	-5.16	112.02	120.80
1	B	59	ASP	CA-CB-CG	5.10	117.70	112.60
1	E	55	HIS	CB-CA-C	5.09	119.11	111.89
1	E	89	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	57	GLU	CB-CG-CD	5.05	121.18	112.60
1	D	117	ASN	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ARG	Sidechain
1	A	72	ARG	Sidechain
1	A	99	ARG	Sidechain
1	B	72	ARG	Sidechain
1	D	72	ARG	Sidechain
1	E	72	ARG	Sidechain
1	E	99	ARG	Sidechain
1	F	99	ARG	Sidechain

## 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	914	0	908	7	0
1	B	929	0	925	13	0
1	C	933	0	936	10	0
1	D	929	0	925	6	0
1	E	936	0	932	5	0
1	F	933	0	920	11	0
2	B	49	0	0	6	0
2	D	49	0	0	2	0
2	E	49	0	0	0	0
3	A	10	0	0	1	0
3	B	14	0	0	1	0
3	C	16	0	0	1	0
3	D	16	0	0	4	0
3	E	21	0	0	0	0
3	F	8	0	0	1	0
All	All	5806	0	5546	49	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 4.

All (49) 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:D:35:ASP:O	3:D:301:HOH:O	1.68	1.09
1:A:72:ARG:HH22	1:C:88:THR:HG21	1.37	0.88
1:B:101:MET:CE	2:B:201:A1JAE:C3	2.52	0.87
1:B:101:MET:HE1	2:B:201:A1JAE:C3	2.05	0.86
1:D:39:LEU:N	3:D:301:HOH:O	2.16	0.78
1:C:51:ILE:HD13	1:C:73:LEU:HB2	1.63	0.78
1:C:88:THR:HG23	3:C:209:HOH:O	1.84	0.77
1:B:42:TYR:CD2	1:B:101:MET:HE2	2.26	0.70
1:B:45:MET:HE3	1:B:48:LYS:HE3	1.79	0.65
1:A:92:LEU:HD11	1:A:119:PRO:HD3	1.80	0.64
1:F:45:MET:HE1	1:F:48:LYS:HE3	1.81	0.62
1:F:45:MET:CE	1:F:48:LYS:HE3	2.31	0.61
1:A:72:ARG:HH22	1:C:88:THR:CG2	2.11	0.60
1:D:36:LEU:C	3:D:301:HOH:O	2.44	0.60
1:B:42:TYR:HD2	1:B:101:MET:HE2	1.65	0.60
1:F:45:MET:HE2	1:F:67:TYR:OH	2.03	0.59
2:B:201:A1JAE:C29	3:B:314:HOH:O	2.50	0.58
1:B:101:MET:HE3	2:B:201:A1JAE:C5	2.36	0.56
1:D:108:ASP:OD1	2:D:201:A1JAE:C1	2.54	0.55
1:B:45:MET:CE	1:B:48:LYS:HE3	2.37	0.54
1:E:26:CYS:SG	1:E:102:ILE:HD11	2.47	0.54
1:C:59:ASP:OD1	1:C:61:LYS:HG2	2.08	0.54
1:F:45:MET:HE1	1:F:48:LYS:CE	2.38	0.54
1:B:101:MET:HE3	2:B:201:A1JAE:C27	2.38	0.53
1:B:18:TYR:HD2	1:B:119:PRO:HG3	1.76	0.50
1:C:100:CYS:SG	1:C:100:CYS:O	2.71	0.48
1:F:45:MET:HE1	1:F:48:LYS:NZ	2.28	0.47
3:A:208:HOH:O	2:D:201:A1JAE:C29	2.63	0.47
1:C:51:ILE:CD1	1:C:73:LEU:HB2	2.41	0.47
1:B:45:MET:HE2	1:B:67:TYR:OH	2.17	0.45
1:F:34:LEU:HD22	1:F:79:SER:N	2.32	0.45
1:F:53:PHE:HE1	1:F:75:LYS:HE3	1.80	0.44
1:F:100:CYS:O	1:F:100:CYS:SG	2.75	0.44
1:B:45:MET:HE1	1:B:48:LYS:NZ	2.33	0.44
1:F:34:LEU:HB2	1:F:79:SER:HA	2.01	0.43
1:F:68:ARG:HG2	1:F:69:GLN:HG3	2.01	0.43
1:E:53:PHE:CE1	1:E:75:LYS:HE2	2.54	0.43
1:A:115:LYS:HB2	1:E:113:THR:HG21	2.01	0.43
1:A:72:ARG:NH2	1:C:88:THR:HG21	2.19	0.43
1:B:101:MET:CE	2:B:201:A1JAE:C4	2.97	0.42
1:C:93:GLN:HB2	3:F:207:HOH:O	2.19	0.42
1:D:39:LEU:CB	3:D:301:HOH:O	2.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:VAL:HG23	1:C:108:ASP:HB3	2.02	0.42
1:E:45:MET:HE2	1:E:67:TYR:OH	2.20	0.42
1:B:18:TYR:CD2	1:B:119:PRO:HG3	2.55	0.41
1:F:45:MET:HE3	1:F:48:LYS:HE3	2.02	0.41
1:A:100:CYS:O	1:A:100:CYS:SG	2.78	0.41
1:A:92:LEU:HG	1:E:111:ARG:NH2	2.35	0.41
1:D:54:VAL:HG12	1:D:55:HIS:CD2	2.57	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 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	114/128 (89%)	111 (97%)	3 (3%)	0	100	100
1	B	115/128 (90%)	112 (97%)	3 (3%)	0	100	100
1	C	115/128 (90%)	111 (96%)	3 (3%)	1 (1%)	14	4
1	D	115/128 (90%)	111 (96%)	4 (4%)	0	100	100
1	E	115/128 (90%)	112 (97%)	3 (3%)	0	100	100
1	F	116/128 (91%)	112 (97%)	4 (3%)	0	100	100
All	All	690/768 (90%)	669 (97%)	20 (3%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	119	PRO

### 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	98/110 (89%)	97 (99%)	1 (1%)	68	56
1	B	100/110 (91%)	99 (99%)	1 (1%)	68	56
1	C	101/110 (92%)	99 (98%)	2 (2%)	48	29
1	D	100/110 (91%)	96 (96%)	4 (4%)	28	9
1	E	101/110 (92%)	97 (96%)	4 (4%)	28	9
1	F	99/110 (90%)	98 (99%)	1 (1%)	68	56
All	All	599/660 (91%)	586 (98%)	13 (2%)	45	26

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	B	45	MET
1	C	51	ILE
1	C	119	PRO
1	D	31	GLU
1	D	33	GLN
1	D	45	MET
1	D	51	ILE
1	E	31	GLU
1	E	45	MET
1	E	58	GLU
1	E	75	LYS
1	F	45	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	55	HIS
1	B	63	GLN
1	C	63	GLN
1	D	33	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	55	HIS
1	D	86	GLN
1	E	55	HIS
1	F	55	HIS

### 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](#)

3 ligands are modelled in this entry.

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$
2	A1JAE	E	201	-	52,52,52	0.73	1 (1%)	71,73,73	2.24	15 (21%)
2	A1JAE	B	201	-	52,52,52	0.71	1 (1%)	71,73,73	2.06	15 (21%)
2	A1JAE	D	201	-	52,52,52	0.62	0	71,73,73	1.63	16 (22%)

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
2	A1JAE	E	201	-	-	17/48/48/48	0/4/4/4
2	A1JAE	B	201	-	-	10/48/48/48	0/4/4/4
2	A1JAE	D	201	-	-	19/48/48/48	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	A1JAE	C5-C27	2.37	1.42	1.39
2	B	201	A1JAE	C5-C27	2.09	1.41	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	A1JAE	C1-O1-C2	11.14	133.86	117.51
2	B	201	A1JAE	C1-O1-C2	11.10	133.80	117.51
2	E	201	A1JAE	O5-C24-C21	6.95	125.81	111.68
2	D	201	A1JAE	C1-O1-C2	6.03	126.36	117.51
2	D	201	A1JAE	O4-C23-C21	4.68	121.21	111.68
2	B	201	A1JAE	O7-C34-C32	4.67	121.18	111.68
2	E	201	A1JAE	C4-C5-C27	4.39	128.95	123.82
2	E	201	A1JAE	C14-C26-CL1	-4.03	116.56	119.50
2	B	201	A1JAE	C3-C4-C5	3.64	126.71	120.61
2	B	201	A1JAE	O5-C24-C21	3.58	118.96	111.68
2	B	201	A1JAE	C13-C14-C26	3.57	121.61	118.81
2	E	201	A1JAE	C35-C32-C33	-3.49	102.37	110.02
2	E	201	A1JAE	O7-C34-C32	3.48	118.77	111.68
2	E	201	A1JAE	C35-C32-C34	3.38	117.43	110.02
2	B	201	A1JAE	O3-C22-C21	3.35	118.49	111.68
2	E	201	A1JAE	C24-C21-C22	-3.34	102.69	110.02
2	E	201	A1JAE	C3-C4-C5	3.31	126.15	120.61
2	B	201	A1JAE	C4-C5-C27	3.22	127.59	123.82
2	D	201	A1JAE	C23-C21-N2	3.19	118.53	109.02
2	D	201	A1JAE	C35-C32-C33	3.12	116.86	110.02
2	D	201	A1JAE	C5-C27-CL2	3.10	122.36	119.67
2	E	201	A1JAE	C24-C21-N2	3.08	118.22	109.02
2	E	201	A1JAE	O8-C35-C32	2.98	117.74	111.68
2	E	201	A1JAE	C9-C27-CL2	-2.96	117.10	119.67
2	D	201	A1JAE	C3-C4-C5	2.86	125.40	120.61
2	D	201	A1JAE	C33-C32-N4	-2.85	100.51	109.02
2	D	201	A1JAE	O7-C34-C32	2.83	117.45	111.68
2	B	201	A1JAE	C24-C21-C23	-2.80	103.89	110.02
2	B	201	A1JAE	O4-C23-C21	2.79	117.36	111.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	A1JAE	C11-C10-C26	-2.68	116.05	119.07
2	E	201	A1JAE	C6-C5-C4	-2.63	113.47	118.70
2	D	201	A1JAE	C34-C32-N4	2.56	116.66	109.02
2	B	201	A1JAE	C30-C31-N4	-2.46	106.27	112.36
2	D	201	A1JAE	C19-C20-N2	-2.46	103.71	111.49
2	E	201	A1JAE	C9-C10-C26	2.46	125.62	122.78
2	B	201	A1JAE	C28-C4-C3	-2.39	114.95	118.23
2	B	201	A1JAE	O6-C33-C32	2.28	116.33	111.68
2	D	201	A1JAE	C6-C5-C4	-2.28	114.17	118.70
2	D	201	A1JAE	C28-C4-C5	-2.24	117.20	120.91
2	D	201	A1JAE	C4-C5-C27	2.24	126.44	123.82
2	B	201	A1JAE	C26-C14-N1	-2.20	115.14	118.64
2	D	201	A1JAE	C24-C21-C23	-2.18	105.23	110.02
2	D	201	A1JAE	C18-C17-C16	-2.16	115.84	118.89
2	B	201	A1JAE	C6-C5-C27	-2.11	116.70	119.07
2	B	201	A1JAE	O8-C35-C32	2.06	115.88	111.68
2	D	201	A1JAE	C9-C27-CL2	-2.00	117.93	119.67

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	A1JAE	C24-C21-C22-O3
2	B	201	A1JAE	N4-C32-C35-O8
2	B	201	A1JAE	C33-C32-C35-O8
2	B	201	A1JAE	C34-C32-C35-O8
2	D	201	A1JAE	C22-C21-N2-C20
2	D	201	A1JAE	C23-C21-N2-C20
2	D	201	A1JAE	C24-C21-N2-C20
2	D	201	A1JAE	N2-C21-C23-O4
2	D	201	A1JAE	C22-C21-C23-O4
2	D	201	A1JAE	C24-C21-C23-O4
2	D	201	A1JAE	N2-C21-C24-O5
2	D	201	A1JAE	C22-C21-C24-O5
2	D	201	A1JAE	C23-C21-C24-O5
2	D	201	A1JAE	C33-C32-N4-C31
2	D	201	A1JAE	C34-C32-N4-C31
2	D	201	A1JAE	C35-C32-N4-C31
2	D	201	A1JAE	N4-C32-C34-O7
2	D	201	A1JAE	C33-C32-C34-O7
2	D	201	A1JAE	C35-C32-C34-O7
2	E	201	A1JAE	C19-C20-N2-C21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	E	201	A1JAE	C33-C32-N4-C31
2	E	201	A1JAE	C34-C32-N4-C31
2	E	201	A1JAE	C35-C32-N4-C31
2	E	201	A1JAE	N4-C32-C34-O7
2	E	201	A1JAE	C33-C32-C34-O7
2	E	201	A1JAE	C35-C32-C34-O7
2	E	201	A1JAE	N4-C32-C35-O8
2	E	201	A1JAE	C33-C32-C35-O8
2	E	201	A1JAE	C34-C32-C35-O8
2	E	201	A1JAE	N1-C15-C16-C17
2	E	201	A1JAE	O2-C15-C16-C17
2	E	201	A1JAE	N1-C15-C16-N3
2	B	201	A1JAE	C30-C2-O1-C1
2	E	201	A1JAE	O2-C15-C16-N3
2	E	201	A1JAE	C30-C2-O1-C1
2	D	201	A1JAE	C30-C2-O1-C1
2	D	201	A1JAE	C3-C2-O1-C1
2	E	201	A1JAE	C3-C2-O1-C1
2	B	201	A1JAE	C3-C2-O1-C1
2	B	201	A1JAE	C19-C20-N2-C21
2	D	201	A1JAE	N4-C32-C33-O6
2	B	201	A1JAE	C23-C21-C22-O3
2	E	201	A1JAE	C24-C21-N2-C20
2	D	201	A1JAE	C19-C20-N2-C21
2	B	201	A1JAE	N2-C21-C22-O3
2	B	201	A1JAE	C28-C4-C5-C27

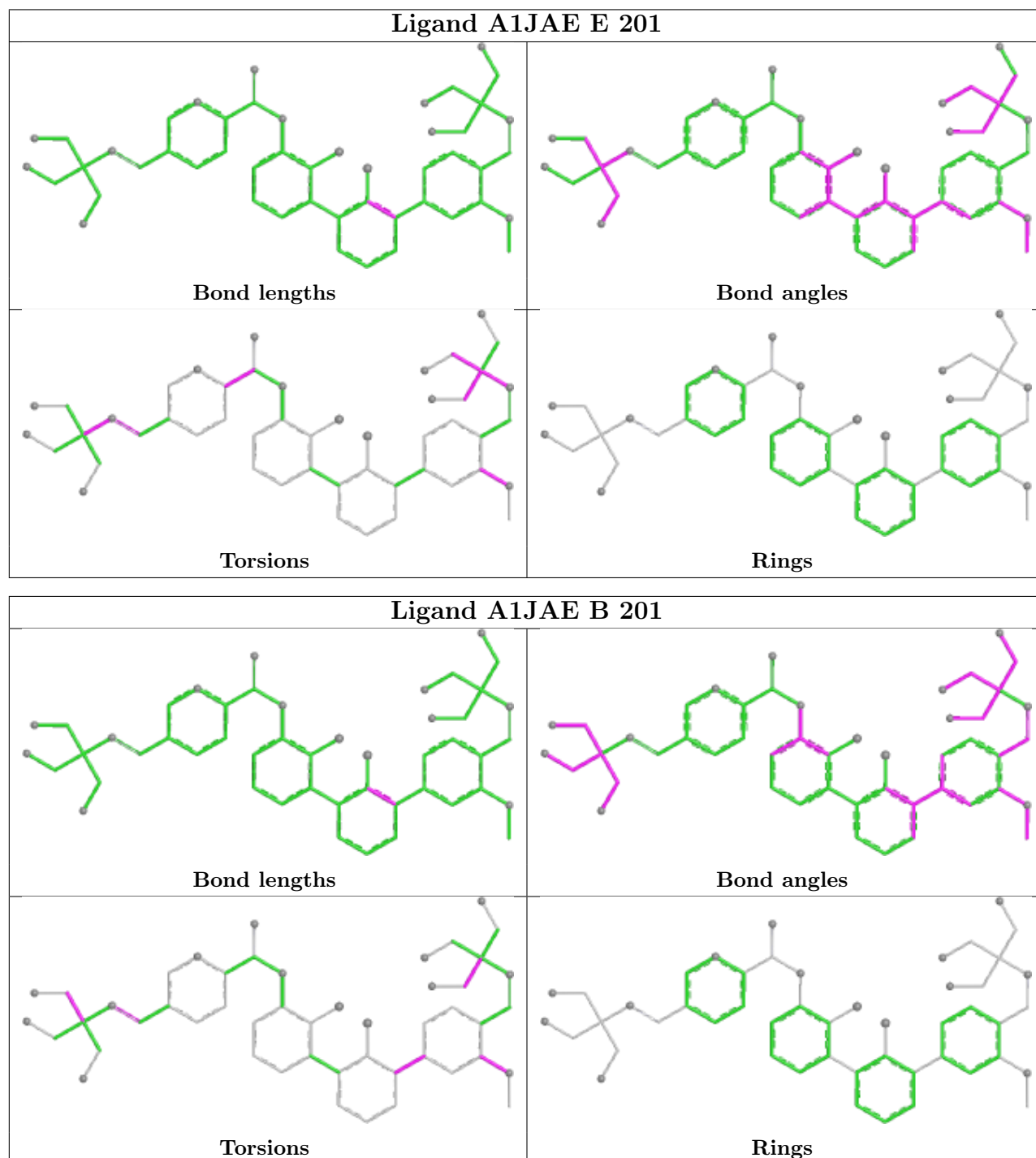
There are no ring outliers.

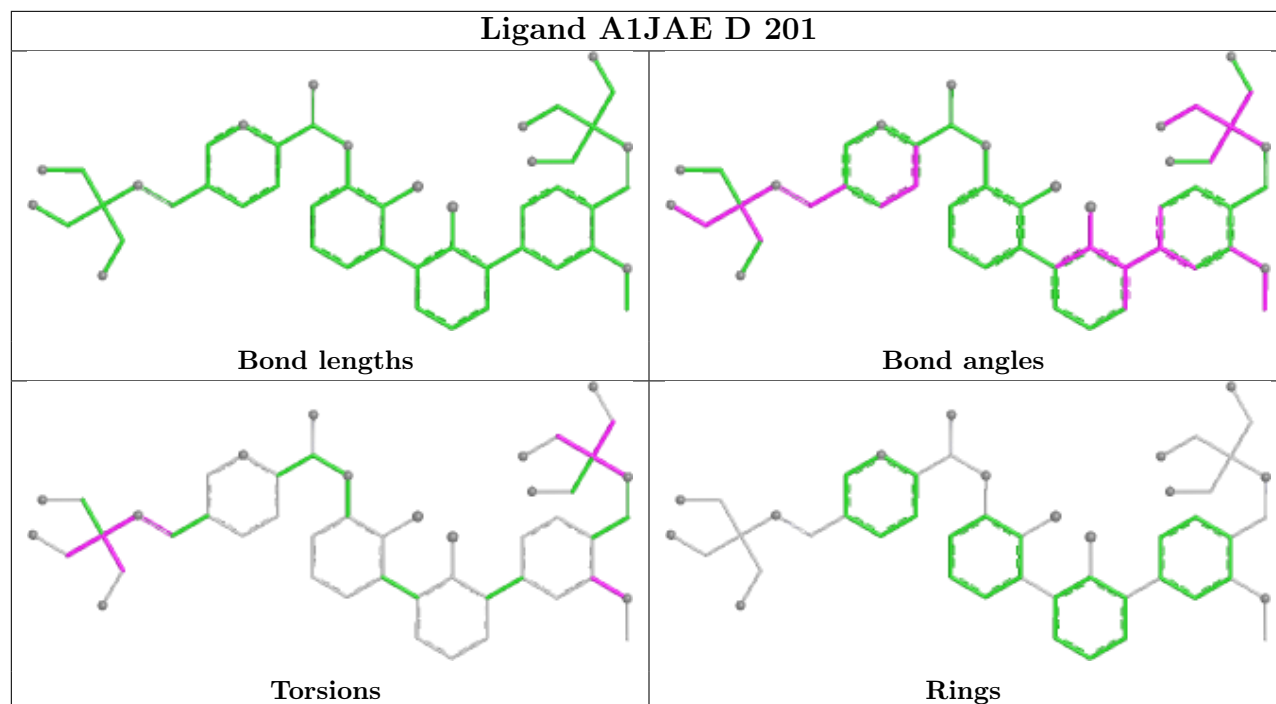
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	A1JAE	6	0
2	D	201	A1JAE	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	116/128 (90%)	1.13	22 (18%) 3 3	21, 33, 67, 88	0
1	B	117/128 (91%)	0.64	7 (5%) 27 31	20, 30, 56, 82	0
1	C	117/128 (91%)	0.74	12 (10%) 12 13	21, 31, 55, 67	0
1	D	117/128 (91%)	0.95	16 (13%) 6 7	22, 34, 63, 74	0
1	E	117/128 (91%)	0.69	10 (8%) 16 20	21, 30, 55, 82	0
1	F	118/128 (92%)	1.18	19 (16%) 4 5	26, 39, 64, 90	0
All	All	702/768 (91%)	0.89	86 (12%) 8 9	20, 33, 62, 90	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	LEU	9.0
1	B	120	TYR	7.5
1	C	120	TYR	6.1
1	D	120	TYR	5.8
1	A	117	ASN	4.6
1	A	118	ALA	4.5
1	A	4	ALA	4.4
1	A	60	LEU	4.4
1	A	116	VAL	4.3
1	D	4	ALA	4.3
1	D	54	VAL	4.3
1	B	55	HIS	4.2
1	E	4	ALA	4.0
1	D	55	HIS	3.9
1	F	74	LEU	3.8
1	E	120	TYR	3.8
1	F	53	PHE	3.7
1	D	30	VAL	3.5
1	B	4	ALA	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	36	LEU	3.4
1	A	91	LYS	3.4
1	F	120	TYR	3.3
1	C	4	ALA	3.3
1	A	18	TYR	3.2
1	F	30	VAL	3.2
1	B	54	VAL	3.2
1	D	34	LEU	3.1
1	A	62	VAL	3.1
1	F	66	SER	3.1
1	A	93	GLN	3.1
1	E	100	CYS	3.0
1	A	32	LYS	2.9
1	F	34	LEU	2.9
1	D	76	ASP	2.9
1	A	55	HIS	2.9
1	C	62	VAL	2.8
1	F	38	ALA	2.8
1	A	119	PRO	2.8
1	D	80	LEU	2.8
1	E	26	CYS	2.7
1	C	74	LEU	2.7
1	F	4	ALA	2.7
1	F	26	CYS	2.6
1	A	65	SER	2.6
1	A	16	VAL	2.6
1	A	36	LEU	2.6
1	B	60	LEU	2.6
1	F	60	LEU	2.5
1	F	78	LEU	2.5
1	D	31	GLU	2.5
1	F	76	ASP	2.5
1	D	79	SER	2.5
1	D	38	ALA	2.5
1	A	79	SER	2.5
1	F	79	SER	2.5
1	D	29	PRO	2.5
1	C	54	VAL	2.5
1	D	75	LYS	2.4
1	A	90	VAL	2.4
1	D	33	GLN	2.3
1	A	95	ALA	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	55	HIS	2.3
1	E	105	GLY	2.3
1	E	32	LYS	2.3
1	F	121	ALA	2.3
1	C	75	LYS	2.3
1	F	24	ILE	2.3
1	E	118	ALA	2.2
1	D	60	LEU	2.2
1	E	76	ASP	2.2
1	F	54	VAL	2.1
1	E	36	LEU	2.1
1	C	66	SER	2.1
1	A	67	TYR	2.1
1	B	61	LYS	2.1
1	E	6	THR	2.1
1	B	51	ILE	2.1
1	F	104	TYR	2.1
1	A	37	ALA	2.0
1	C	65	SER	2.0
1	D	72	ARG	2.0
1	C	60	LEU	2.0
1	F	55	HIS	2.0
1	C	32	LYS	2.0
1	A	15	VAL	2.0
1	C	26	CYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

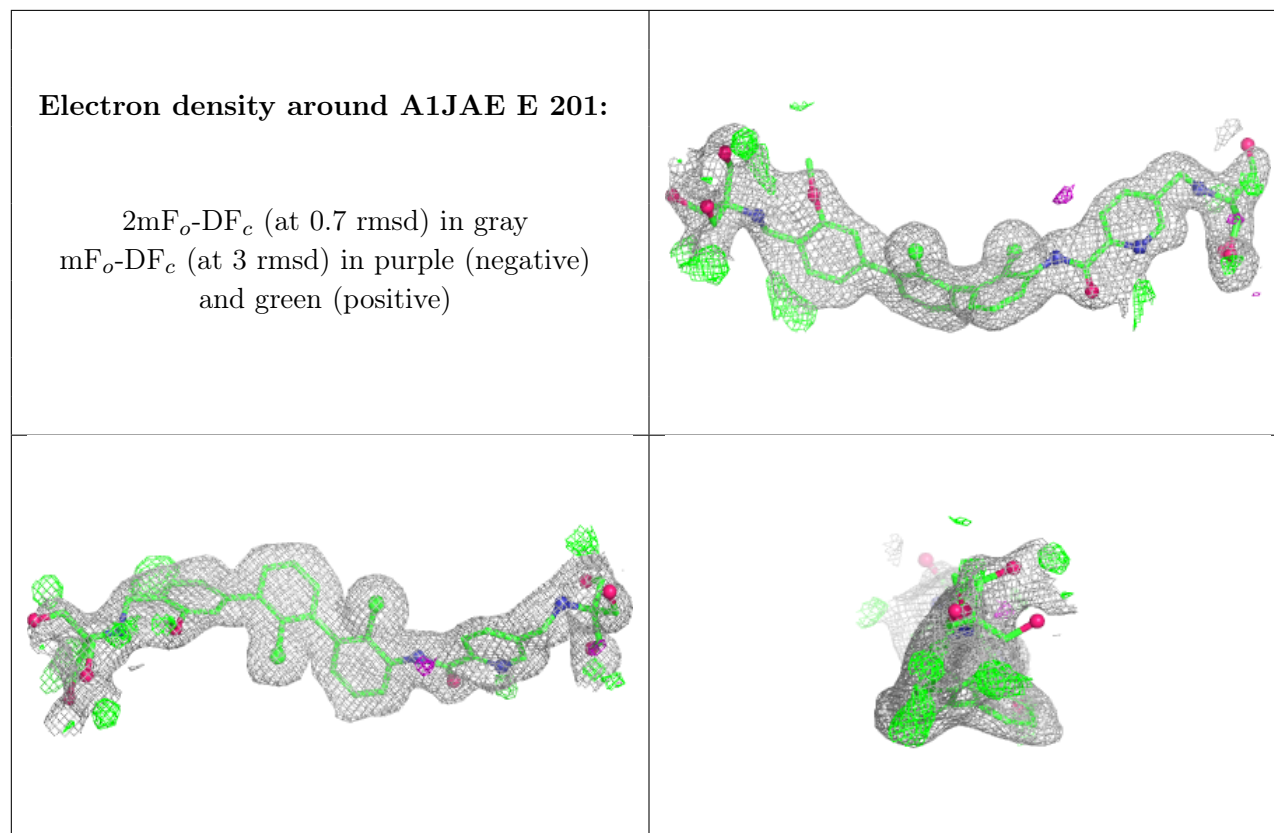
There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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.

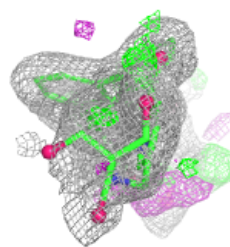
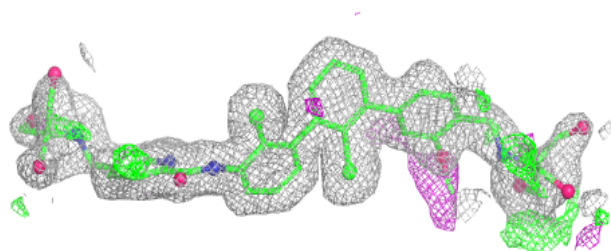
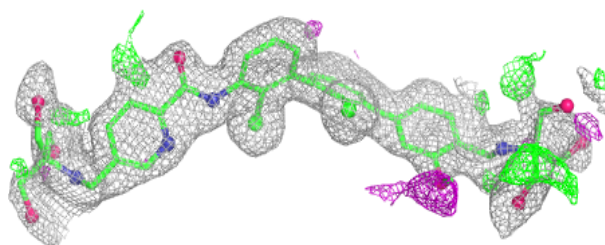
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A1JAE	E	201	49/49	0.91	0.13	23,36,67,78	0
2	A1JAE	D	201	49/49	0.92	0.13	17,34,65,76	0
2	A1JAE	B	201	49/49	0.92	0.14	16,35,73,85	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

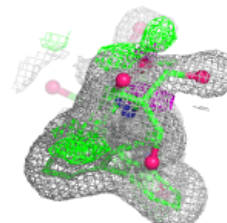
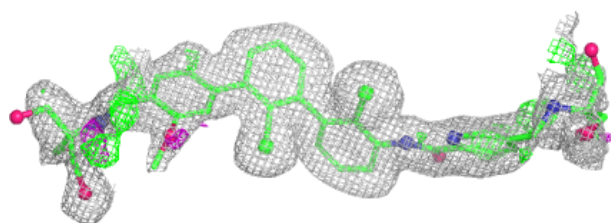
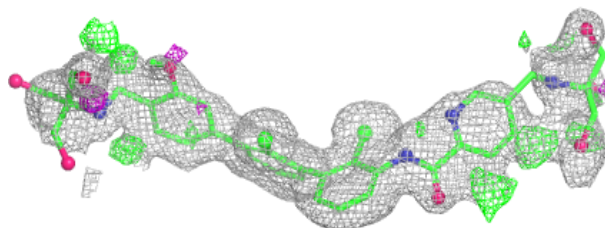


**Electron density around A1JAE D 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around A1JAE B 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.