



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 11:32 AM EST

PDB ID : 5T5O  
Title : LECTIN FROM BAUHINIA FORFICATA IN COMPLEX WITH TN-  
PEPTIDE  
Authors : Lubkowski, J.; Wlodawer, A.  
Deposited on : 2016-08-31  
Resolution : 2.75 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

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  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

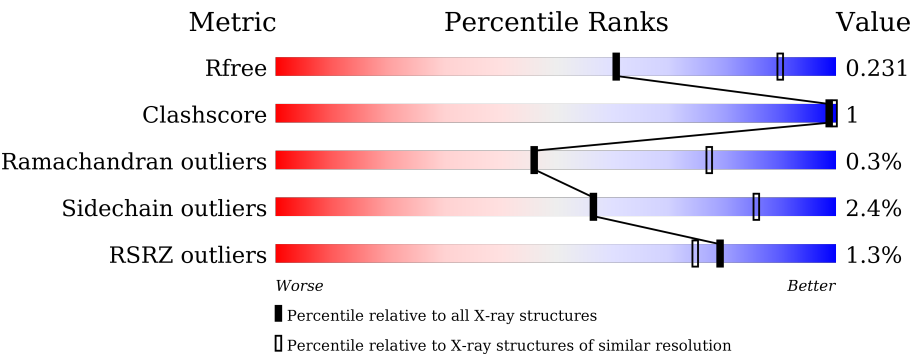
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	242	<div><div></div><div>88%5% • 5%</div></div>
1	B	242	<div><div></div><div>84%9% • 5%</div></div>
1	C	242	<div><div></div><div>90%5% 5%</div></div>
1	D	242	<div><div>%</div><div>89%5% • 5%</div></div>
1	E	242	<div><div></div><div>89%6% 5%</div></div>
1	F	242	<div><div></div><div>89%5% • 5%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	242	<div><div></div><div>2%</div><div>91%</div><div>5%</div></div>
1	H	242	<div><div></div><div>2%</div><div>91%</div><div>5%</div></div>
1	I	242	<div><div></div><div>2%</div><div>90%</div><div>5%</div><div>5%</div></div>
1	J	242	<div><div></div><div>3%</div><div>90%</div><div>5%</div><div>5%</div></div>
2	a	6	<div><div></div><div>83%</div><div>17%</div></div>
2	b	6	<div><div></div><div>83%</div><div>17%</div></div>
2	c	6	<div><div></div><div>17%</div><div>83%</div><div>17%</div></div>
2	d	6	<div><div></div><div>67%</div><div>33%</div></div>
2	e	6	<div><div></div><div>17%</div><div>83%</div><div>17%</div></div>
2	f	6	<div><div></div><div>67%</div><div>17%</div><div>17%</div></div>
2	g	6	<div><div></div><div>83%</div><div>17%</div></div>
2	h	6	<div><div></div><div>100%</div></div>
2	i	6	<div><div></div><div>17%</div><div>100%</div></div>
2	j	6	<div><div></div><div>17%</div><div>83%</div><div>17%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18803 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 Lectin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	0	0	0
			1811	1156	305	350			
1	B	229	Total	C	N	O	0	0	0
			1811	1156	305	350			
1	C	229	Total	C	N	O	0	0	0
			1811	1156	305	350			
1	D	229	Total	C	N	O	0	0	0
			1811	1156	305	350			
1	E	229	Total	C	N	O	0	0	0
			1811	1156	305	350			
1	F	229	Total	C	N	O	0	0	0
			1811	1156	305	350			
1	G	229	Total	C	N	O	0	0	0
			1811	1156	305	350			
1	H	229	Total	C	N	O	0	0	0
			1811	1156	305	350			
1	I	229	Total	C	N	O	0	0	0
			1811	1156	305	350			
1	J	229	Total	C	N	O	0	0	0
			1811	1156	305	350			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	GLY	-	expression tag	UNP P86993
A	235	ALA	-	expression tag	UNP P86993
A	236	ARG	-	expression tag	UNP P86993
A	237	HIS	-	expression tag	UNP P86993
A	238	HIS	-	expression tag	UNP P86993
A	239	HIS	-	expression tag	UNP P86993
A	240	HIS	-	expression tag	UNP P86993
A	241	HIS	-	expression tag	UNP P86993
A	242	HIS	-	expression tag	UNP P86993

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Chain	Residue	Modelled	Actual	Comment	Reference
B	234	GLY	-	expression tag	UNP P86993
B	235	ALA	-	expression tag	UNP P86993
B	236	ARG	-	expression tag	UNP P86993
B	237	HIS	-	expression tag	UNP P86993
B	238	HIS	-	expression tag	UNP P86993
B	239	HIS	-	expression tag	UNP P86993
B	240	HIS	-	expression tag	UNP P86993
B	241	HIS	-	expression tag	UNP P86993
B	242	HIS	-	expression tag	UNP P86993
C	234	GLY	-	expression tag	UNP P86993
C	235	ALA	-	expression tag	UNP P86993
C	236	ARG	-	expression tag	UNP P86993
C	237	HIS	-	expression tag	UNP P86993
C	238	HIS	-	expression tag	UNP P86993
C	239	HIS	-	expression tag	UNP P86993
C	240	HIS	-	expression tag	UNP P86993
C	241	HIS	-	expression tag	UNP P86993
C	242	HIS	-	expression tag	UNP P86993
D	234	GLY	-	expression tag	UNP P86993
D	235	ALA	-	expression tag	UNP P86993
D	236	ARG	-	expression tag	UNP P86993
D	237	HIS	-	expression tag	UNP P86993
D	238	HIS	-	expression tag	UNP P86993
D	239	HIS	-	expression tag	UNP P86993
D	240	HIS	-	expression tag	UNP P86993
D	241	HIS	-	expression tag	UNP P86993
D	242	HIS	-	expression tag	UNP P86993
E	234	GLY	-	expression tag	UNP P86993
E	235	ALA	-	expression tag	UNP P86993
E	236	ARG	-	expression tag	UNP P86993
E	237	HIS	-	expression tag	UNP P86993
E	238	HIS	-	expression tag	UNP P86993
E	239	HIS	-	expression tag	UNP P86993
E	240	HIS	-	expression tag	UNP P86993
E	241	HIS	-	expression tag	UNP P86993
E	242	HIS	-	expression tag	UNP P86993
F	234	GLY	-	expression tag	UNP P86993
F	235	ALA	-	expression tag	UNP P86993
F	236	ARG	-	expression tag	UNP P86993
F	237	HIS	-	expression tag	UNP P86993
F	238	HIS	-	expression tag	UNP P86993
F	239	HIS	-	expression tag	UNP P86993

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Chain	Residue	Modelled	Actual	Comment	Reference
F	240	HIS	-	expression tag	UNP P86993
F	241	HIS	-	expression tag	UNP P86993
F	242	HIS	-	expression tag	UNP P86993
G	234	GLY	-	expression tag	UNP P86993
G	235	ALA	-	expression tag	UNP P86993
G	236	ARG	-	expression tag	UNP P86993
G	237	HIS	-	expression tag	UNP P86993
G	238	HIS	-	expression tag	UNP P86993
G	239	HIS	-	expression tag	UNP P86993
G	240	HIS	-	expression tag	UNP P86993
G	241	HIS	-	expression tag	UNP P86993
G	242	HIS	-	expression tag	UNP P86993
H	234	GLY	-	expression tag	UNP P86993
H	235	ALA	-	expression tag	UNP P86993
H	236	ARG	-	expression tag	UNP P86993
H	237	HIS	-	expression tag	UNP P86993
H	238	HIS	-	expression tag	UNP P86993
H	239	HIS	-	expression tag	UNP P86993
H	240	HIS	-	expression tag	UNP P86993
H	241	HIS	-	expression tag	UNP P86993
H	242	HIS	-	expression tag	UNP P86993
I	234	GLY	-	expression tag	UNP P86993
I	235	ALA	-	expression tag	UNP P86993
I	236	ARG	-	expression tag	UNP P86993
I	237	HIS	-	expression tag	UNP P86993
I	238	HIS	-	expression tag	UNP P86993
I	239	HIS	-	expression tag	UNP P86993
I	240	HIS	-	expression tag	UNP P86993
I	241	HIS	-	expression tag	UNP P86993
I	242	HIS	-	expression tag	UNP P86993
J	234	GLY	-	expression tag	UNP P86993
J	235	ALA	-	expression tag	UNP P86993
J	236	ARG	-	expression tag	UNP P86993
J	237	HIS	-	expression tag	UNP P86993
J	238	HIS	-	expression tag	UNP P86993
J	239	HIS	-	expression tag	UNP P86993
J	240	HIS	-	expression tag	UNP P86993
J	241	HIS	-	expression tag	UNP P86993
J	242	HIS	-	expression tag	UNP P86993

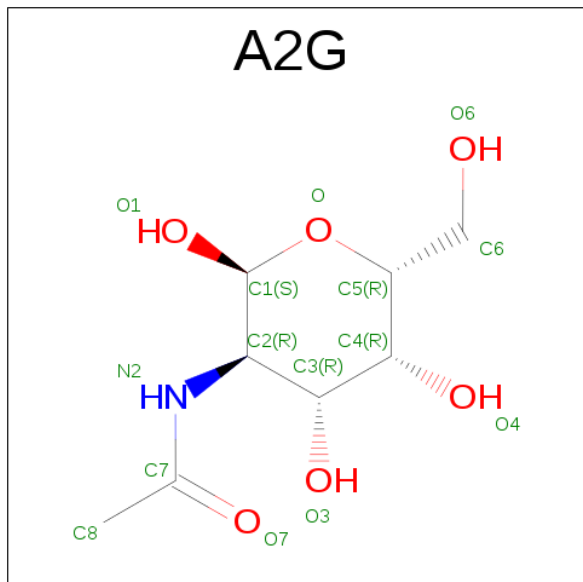
- Molecule 2 is a protein called TN-peptide ACE-GLY-VAL-THR-SER-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	a	6	Total	C	N	O	0	0	0
			32	19	5	8			
2	b	6	Total	C	N	O	0	0	0
			32	19	5	8			
2	c	6	Total	C	N	O	0	0	0
			32	19	5	8			
2	d	6	Total	C	N	O	0	0	0
			32	19	5	8			
2	e	6	Total	C	N	O	0	0	0
			32	19	5	8			
2	f	6	Total	C	N	O	0	0	0
			32	19	5	8			
2	g	6	Total	C	N	O	0	0	0
			32	19	5	8			
2	h	6	Total	C	N	O	0	0	0
			32	19	5	8			
2	i	6	Total	C	N	O	0	0	0
			32	19	5	8			
2	j	6	Total	C	N	O	0	0	0
			32	19	5	8			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total	Ca	0	0
			2	2		
3	J	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		
3	E	2	Total	Ca	0	0
			2	2		
3	H	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		
3	I	2	Total	Ca	0	0
			2	2		
3	C	2	Total	Ca	0	0
			2	2		
3	A	2	Total	Ca	0	0
			2	2		
3	F	2	Total	Ca	0	0
			2	2		

- Molecule 4 is N-ACETYL-2-DEOXY-2-AMINO-GALACTOSE (three-letter code: A2G) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	a	1	Total	C	N	O	0	0
			14	8	1	5		
4	b	1	Total	C	N	O	0	0
			14	8	1	5		
4	c	1	Total	C	N	O	0	0
			14	8	1	5		
4	d	1	Total	C	N	O	0	0
			14	8	1	5		
4	e	1	Total	C	N	O	0	0
			14	8	1	5		
4	f	1	Total	C	N	O	0	0
			14	8	1	5		
4	g	1	Total	C	N	O	0	0
			14	8	1	5		
4	h	1	Total	C	N	O	0	0
			14	8	1	5		
4	i	1	Total	C	N	O	0	0
			14	8	1	5		
4	j	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total 27	O 27	0	0
5	a	1	Total 1	O 1	0	0
5	B	30	Total 30	O 30	0	0
5	b	1	Total 1	O 1	0	0
5	C	18	Total 18	O 18	0	0
5	D	29	Total 29	O 29	0	0
5	E	16	Total 16	O 16	0	0
5	F	26	Total 26	O 26	0	0
5	f	3	Total 3	O 3	0	0
5	G	16	Total 16	O 16	0	0
5	H	18	Total 18	O 18	0	0
5	h	1	Total 1	O 1	0	0
5	I	13	Total 13	O 13	0	0
5	i	1	Total 1	O 1	0	0
5	J	13	Total 13	O 13	0	0

### 3 Residue-property plots [i](#)


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 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.

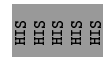
#### • Molecule 1: Lectin

Chain A: 



#### • Molecule 1: Lectin

Chain B: 



#### • Molecule 1: Lectin

Chain C: 



#### • Molecule 1: Lectin

Chain D: 




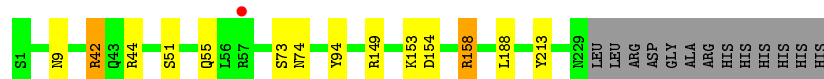
#### • Molecule 1: Lectin

Chain E: 



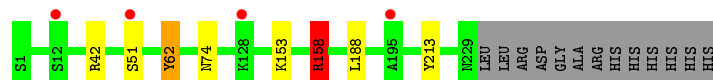
#### • Molecule 1: Lectin

Chain F:  89% 5% • 5%



• Molecule 1: Lectin

Chain G:  91% 2% • 5%




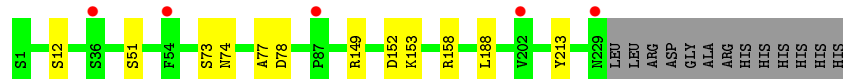
• Molecule 1: Lectin

Chain H:  91% 2% • 5%




• Molecule 1: Lectin

Chain I:  90% 2% 5% 5%




• Molecule 1: Lectin

Chain J:  90% 3% 5% 5%




• Molecule 2: TN-peptide ACE-GLY-VAL-THR-SER-ALA

Chain a:  83% 17%




• Molecule 2: TN-peptide ACE-GLY-VAL-THR-SER-ALA

Chain b:  83% 17%



• Molecule 2: TN-peptide ACE-GLY-VAL-THR-SER-ALA

Chain c:  17% 83% 17%



- Molecule 2: TN-peptide ACE-GLY-VAL-THR-SER-ALA

Chain d: 67% 33%



- Molecule 2: TN-peptide ACE-GLY-VAL-THR-SER-ALA

Chain e: 17% 83% 17%



- Molecule 2: TN-peptide ACE-GLY-VAL-THR-SER-ALA

Chain f: 67% 17% 17%



- Molecule 2: TN-peptide ACE-GLY-VAL-THR-SER-ALA

Chain g: 83% 17%



- Molecule 2: TN-peptide ACE-GLY-VAL-THR-SER-ALA

Chain h: 100%

There are no outlier residues recorded for this chain.

- Molecule 2: TN-peptide ACE-GLY-VAL-THR-SER-ALA

Chain i: 17% 100%



- Molecule 2: TN-peptide ACE-GLY-VAL-THR-SER-ALA

Chain j: 17% 83% 17%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.08Å 187.29Å 258.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 2.75 49.38 – 2.70	Depositor EDS
% Data completeness (in resolution range)	79.7 (49.38-2.75) 81.3 (49.38-2.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.96 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.201 , 0.230 0.203 , 0.231	Depositor DCC
$R_{free}$ test set	3444 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.6	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 33.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18803	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: CA, ACE, A2G

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	1.22	4/1864 (0.2%)	1.11	10/2547 (0.4%)
1	B	1.26	12/1864 (0.6%)	1.08	13/2547 (0.5%)
1	C	0.88	0/1864	0.89	3/2547 (0.1%)
1	D	1.06	4/1864 (0.2%)	0.99	4/2547 (0.2%)
1	E	0.85	0/1864	0.90	7/2547 (0.3%)
1	F	0.98	1/1864 (0.1%)	0.99	8/2547 (0.3%)
1	G	0.81	1/1864 (0.1%)	0.87	2/2547 (0.1%)
1	H	0.95	0/1864	0.94	2/2547 (0.1%)
1	I	0.81	0/1864	0.87	3/2547 (0.1%)
1	J	0.81	0/1864	0.87	1/2547 (0.0%)
2	a	1.59	0/29	1.53	0/39
2	b	1.96	1/29 (3.4%)	1.29	0/39
2	c	1.36	0/29	1.17	0/39
2	d	1.80	1/29 (3.4%)	1.42	0/39
2	e	1.69	1/29 (3.4%)	1.17	0/39
2	f	1.98	1/29 (3.4%)	1.33	0/39
2	g	1.52	0/29	1.07	0/39
2	h	1.49	0/29	1.30	0/39
2	i	1.49	0/29	1.11	0/39
2	j	1.56	0/29	1.17	0/39
All	All	0.99	26/18930 (0.1%)	0.96	53/25860 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	c	0	1
2	d	0	1
2	f	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	j	0	1
All	All	0	4

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	GLU	CG-CD	10.23	1.67	1.51
1	A	44	ARG	CZ-NH1	7.99	1.43	1.33
1	D	213	TYR	CE1-CZ	7.22	1.48	1.38
1	B	224	SER	CB-OG	7.04	1.51	1.42
1	B	102	GLU	CD-OE1	6.95	1.33	1.25
1	B	104	ASN	CB-CG	-6.93	1.35	1.51
1	A	44	ARG	NE-CZ	6.69	1.41	1.33
1	B	102	GLU	CD-OE2	6.62	1.32	1.25
1	F	73	SER	CB-OG	-6.17	1.34	1.42
1	B	126	GLU	CD-OE1	6.04	1.32	1.25
1	D	74	ASN	CB-CG	-5.85	1.37	1.51
2	d	105	ALA	CA-CB	5.75	1.64	1.52
1	A	214	GLU	CD-OE2	5.72	1.31	1.25
1	A	126	GLU	CD-OE2	5.63	1.31	1.25
1	D	213	TYR	CG-CD2	5.53	1.46	1.39
2	e	105	ALA	N-CA	5.45	1.57	1.46
1	B	222	SER	CB-OG	-5.38	1.35	1.42
1	B	57	ARG	CZ-NH1	5.37	1.40	1.33
2	f	105	ALA	N-CA	5.36	1.57	1.46
1	B	200	GLY	C-O	-5.25	1.15	1.23
1	B	14	GLU	CG-CD	5.10	1.59	1.51
1	D	88	ASP	CB-CG	5.09	1.62	1.51
1	G	62	TYR	CE1-CZ	5.05	1.45	1.38
1	B	19	GLN	CD-NE2	5.05	1.45	1.32
1	B	88	ASP	CB-CG	5.03	1.62	1.51
2	b	101	GLY	N-CA	5.00	1.53	1.46

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ARG	NE-CZ-NH1	14.75	127.67	120.30
1	A	44	ARG	NE-CZ-NH2	-10.33	115.14	120.30
1	F	74	ASN	CB-CA-C	-8.68	93.05	110.40
1	B	74	ASN	CB-CA-C	-8.09	94.21	110.40
1	A	88	ASP	CB-CG-OD2	-7.79	111.28	118.30
1	A	158	ARG	NE-CZ-NH1	7.49	124.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	74	ASN	CB-CA-C	-7.49	95.43	110.40
1	B	78	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	15	ASP	CB-CG-OD2	7.33	124.90	118.30
1	D	74	ASN	CB-CA-C	-7.32	95.77	110.40
1	B	57	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	G	74	ASN	CB-CA-C	-7.29	95.82	110.40
1	A	42	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	74	ASN	CB-CA-C	-7.14	96.12	110.40
1	B	44	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	J	74	ASN	CB-CA-C	-6.90	96.61	110.40
1	B	102	GLU	OE1-CD-OE2	-6.67	115.29	123.30
1	A	57	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	E	74	ASN	CB-CA-C	-6.57	97.27	110.40
1	B	88	ASP	CB-CG-OD1	6.40	124.06	118.30
1	F	154	ASP	CB-CG-OD1	6.21	123.89	118.30
1	F	44	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	C	74	ASN	CB-CA-C	-6.15	98.10	110.40
1	B	182	ASP	CB-CG-OD1	6.12	123.81	118.30
1	D	158	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	B	158	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	B	42	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	I	74	ASN	CB-CA-C	-5.88	98.63	110.40
1	F	158	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	H	88	ASP	CB-CG-OD1	5.86	123.57	118.30
1	C	42	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	I	149	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	D	57	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	78	ASP	CB-CG-OD1	5.74	123.47	118.30
1	E	154	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	57	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	F	42	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	152	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	188	LEU	CB-CA-C	-5.57	99.61	110.20
1	A	188	LEU	CB-CA-C	-5.56	99.64	110.20
1	E	42	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	E	146	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	F	44	ARG	CG-CD-NE	-5.35	100.56	111.80
1	D	57	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	I	152	ASP	CB-CG-OD1	5.17	122.96	118.30
1	G	158	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	138	ASP	CB-CG-OD1	5.08	122.87	118.30
1	E	193	ASP	CB-CG-OD1	5.08	122.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	44	ARG	CG-CD-NE	-5.03	101.24	111.80
1	F	154	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	F	149	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	E	25	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	c	104	SER	Peptide
2	d	104	SER	Peptide
2	f	104	SER	Peptide
2	j	104	SER	Peptide

## 5.2 Too-close contacts [i](#)

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	1811	0	1718	0	0
1	B	1811	0	1718	3	0
1	C	1811	0	1718	3	2
1	D	1811	0	1718	4	0
1	E	1811	0	1718	1	0
1	F	1811	0	1718	4	0
1	G	1811	0	1718	4	0
1	H	1811	0	1718	1	0
1	I	1811	0	1718	3	0
1	J	1811	0	1718	4	0
2	a	32	0	31	0	0
2	b	32	0	31	0	0
2	c	32	0	31	0	0
2	d	32	0	31	0	0
2	e	32	0	31	0	0
2	f	32	0	31	0	0
2	g	32	0	31	0	0
2	h	32	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	i	32	0	31	0	0
2	j	32	0	31	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
4	a	14	0	13	0	0
4	b	14	0	13	0	0
4	c	14	0	13	0	0
4	d	14	0	13	0	0
4	e	14	0	13	0	0
4	f	14	0	13	0	0
4	g	14	0	13	0	0
4	h	14	0	13	0	0
4	i	14	0	13	0	0
4	j	14	0	13	0	0
5	A	27	0	0	0	0
5	B	30	0	0	0	0
5	C	18	0	0	0	0
5	D	29	0	0	1	0
5	E	16	0	0	0	0
5	F	26	0	0	0	0
5	G	16	0	0	1	0
5	H	18	0	0	0	0
5	I	13	0	0	1	0
5	J	13	0	0	1	0
5	a	1	0	0	0	0
5	b	1	0	0	0	0
5	f	3	0	0	0	0
5	h	1	0	0	0	0
5	i	1	0	0	0	0
All	All	18803	0	17620	20	2

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 1.

All (20) 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:J:144:SER:OG	5:J:401:HOH:O	2.11	0.68
1:G:42:ARG:NH1	1:J:213:TYR:OH	2.34	0.60
1:D:57:ARG:HH22	1:F:55:GLN:HE22	1.56	0.53
1:C:55:GLN:NE2	1:C:201:ASP:OD1	2.41	0.53
1:G:62:TYR:HB2	1:H:187:VAL:CG2	2.40	0.51
1:C:42:ARG:NH1	1:I:213:TYR:OH	2.44	0.51
1:B:213:TYR:OH	1:F:42:ARG:NH1	2.49	0.45
1:I:73:SER:HB2	5:I:411:HOH:O	2.17	0.44
1:F:9:ASN:OD1	1:F:9:ASN:C	2.56	0.43
1:C:118:GLU:OE1	1:C:138:ASP:OD2	2.36	0.43
1:G:158:ARG:NH1	5:G:402:HOH:O	2.51	0.43
1:D:119:PHE:CD1	1:D:119:PHE:N	2.87	0.42
1:D:70:ARG:NH2	5:D:401:HOH:O	2.29	0.42
1:J:77:ALA:HA	1:J:78:ASP:HA	1.84	0.41
1:E:77:ALA:HA	1:E:78:ASP:HA	1.90	0.41
1:I:77:ALA:HA	1:I:78:ASP:HA	1.90	0.41
1:B:42:ARG:NH1	1:F:213:TYR:OH	2.54	0.41
1:B:118:GLU:OE1	1:B:138:ASP:OD2	2.38	0.40
1:G:213:TYR:OH	1:J:42:ARG:NH1	2.54	0.40
1:D:210:THR:HB	1:D:211:GLY:C	2.42	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:SER:CA	1:C:55:GLN:OE1[4_555]	1.90	0.30
1:C:36:SER:CB	1:C:55:GLN:OE1[4_555]	2.04	0.16

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	227/242 (94%)	215 (95%)	11 (5%)	1 (0%)	39 72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	227/242 (94%)	214 (94%)	12 (5%)	1 (0%)	39	72
1	C	227/242 (94%)	215 (95%)	12 (5%)	0	100	100
1	D	227/242 (94%)	215 (95%)	11 (5%)	1 (0%)	39	72
1	E	227/242 (94%)	218 (96%)	9 (4%)	0	100	100
1	F	227/242 (94%)	217 (96%)	9 (4%)	1 (0%)	39	72
1	G	227/242 (94%)	216 (95%)	11 (5%)	0	100	100
1	H	227/242 (94%)	217 (96%)	9 (4%)	1 (0%)	39	72
1	I	227/242 (94%)	217 (96%)	10 (4%)	0	100	100
1	J	227/242 (94%)	216 (95%)	10 (4%)	1 (0%)	39	72
2	a	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
2	b	4/6 (67%)	4 (100%)	0	0	100	100
2	c	4/6 (67%)	4 (100%)	0	0	100	100
2	d	4/6 (67%)	4 (100%)	0	0	100	100
2	e	4/6 (67%)	2 (50%)	2 (50%)	0	100	100
2	f	4/6 (67%)	4 (100%)	0	0	100	100
2	g	4/6 (67%)	3 (75%)	0	1 (25%)	0	0
2	h	4/6 (67%)	4 (100%)	0	0	100	100
2	i	4/6 (67%)	2 (50%)	2 (50%)	0	100	100
2	j	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
All	All	2310/2480 (93%)	2193 (95%)	110 (5%)	7 (0%)	46	77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	TYR
1	B	94	TYR
1	D	94	TYR
1	H	94	TYR
2	g	104	SER
1	F	94	TYR
1	J	94	TYR

### 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	198/209 (95%)	193 (98%)	5 (2%)	55	85
1	B	198/209 (95%)	193 (98%)	5 (2%)	55	85
1	C	198/209 (95%)	194 (98%)	4 (2%)	63	89
1	D	198/209 (95%)	193 (98%)	5 (2%)	55	85
1	E	198/209 (95%)	193 (98%)	5 (2%)	55	85
1	F	198/209 (95%)	194 (98%)	4 (2%)	63	89
1	G	198/209 (95%)	194 (98%)	4 (2%)	63	89
1	H	198/209 (95%)	194 (98%)	4 (2%)	63	89
1	I	198/209 (95%)	193 (98%)	5 (2%)	55	85
1	J	198/209 (95%)	193 (98%)	5 (2%)	55	85
2	a	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	b	3/3 (100%)	3 (100%)	0	100	100
2	c	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	d	3/3 (100%)	3 (100%)	0	100	100
2	e	3/3 (100%)	3 (100%)	0	100	100
2	f	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	g	3/3 (100%)	3 (100%)	0	100	100
2	h	3/3 (100%)	3 (100%)	0	100	100
2	i	3/3 (100%)	3 (100%)	0	100	100
2	j	3/3 (100%)	3 (100%)	0	100	100
All	All	2010/2120 (95%)	1961 (98%)	49 (2%)	57	86

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	148	THR
1	A	153	LYS

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Mol	Chain	Res	Type
1	A	158	ARG
1	A	188	LEU
2	a	104	SER
1	B	12	SER
1	B	51	SER
1	B	153	LYS
1	B	158	ARG
1	B	188	LEU
1	C	51	SER
1	C	153	LYS
1	C	158	ARG
1	C	188	LEU
2	c	104	SER
1	D	12	SER
1	D	51	SER
1	D	153	LYS
1	D	158	ARG
1	D	188	LEU
1	E	51	SER
1	E	153	LYS
1	E	158	ARG
1	E	188	LEU
1	E	196	GLU
1	F	51	SER
1	F	153	LYS
1	F	158	ARG
1	F	188	LEU
2	f	104	SER
1	G	51	SER
1	G	153	LYS
1	G	158	ARG
1	G	188	LEU
1	H	51	SER
1	H	153	LYS
1	H	158	ARG
1	H	188	LEU
1	I	12	SER
1	I	51	SER
1	I	153	LYS
1	I	158	ARG
1	I	188	LEU
1	J	12	SER

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Mol	Chain	Res	Type
1	J	51	SER
1	J	153	LYS
1	J	158	ARG
1	J	188	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	26	ASN
1	F	55	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 20 are monoatomic - leaving 10 for Mogul analysis.

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
4	A2G	a	201	2	14,14,15	0.99	1 (7%)	15,19,21	3.08	7 (46%)
4	A2G	b	201	2	14,14,15	1.15	1 (7%)	15,19,21	1.83	4 (26%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	A2G	c	201	2	14,14,15	0.73	0	15,19,21	1.53	3 (20%)
4	A2G	d	201	2	14,14,15	1.39	3 (21%)	15,19,21	2.05	4 (26%)
4	A2G	e	201	2	14,14,15	0.71	0	15,19,21	2.39	3 (20%)
4	A2G	f	201	2	14,14,15	0.95	0	15,19,21	1.98	5 (33%)
4	A2G	g	201	2	14,14,15	0.70	0	15,19,21	1.25	3 (20%)
4	A2G	h	201	2	14,14,15	0.86	0	15,19,21	2.24	7 (46%)
4	A2G	i	201	2	14,14,15	1.36	1 (7%)	15,19,21	1.76	5 (33%)
4	A2G	j	201	2	14,14,15	0.66	0	15,19,21	2.04	3 (20%)

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
4	A2G	a	201	2	-	0/6/23/26	0/1/1/1
4	A2G	b	201	2	-	0/6/23/26	0/1/1/1
4	A2G	c	201	2	-	0/6/23/26	0/1/1/1
4	A2G	d	201	2	-	0/6/23/26	0/1/1/1
4	A2G	e	201	2	-	0/6/23/26	0/1/1/1
4	A2G	f	201	2	-	0/6/23/26	0/1/1/1
4	A2G	g	201	2	-	0/6/23/26	0/1/1/1
4	A2G	h	201	2	-	0/6/23/26	0/1/1/1
4	A2G	i	201	2	-	0/6/23/26	0/1/1/1
4	A2G	j	201	2	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	i	201	A2G	C1-C2	-3.48	1.47	1.52
4	a	201	A2G	C1-C2	-2.81	1.48	1.52
4	d	201	A2G	O-C1	-2.69	1.39	1.43
4	d	201	A2G	C1-C2	-2.60	1.48	1.52
4	b	201	A2G	C3-C2	-2.55	1.46	1.52
4	d	201	A2G	C2-N2	-2.29	1.42	1.46

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	e	201	A2G	O-C5-C4	-6.18	99.90	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	201	A2G	C3-C4-C5	-3.82	103.41	110.23
4	a	201	A2G	C4-C3-C2	-3.73	105.55	111.34
4	h	201	A2G	C4-C3-C2	-3.57	105.80	111.34
4	b	201	A2G	O6-C6-C5	-3.47	99.73	111.30
4	f	201	A2G	C3-C4-C5	-3.13	104.64	110.23
4	i	201	A2G	O-C5-C4	-3.08	105.03	110.13
4	d	201	A2G	C8-C7-N2	-3.08	110.20	116.10
4	b	201	A2G	C3-C4-C5	-3.06	104.78	110.23
4	j	201	A2G	O7-C7-C8	-3.00	116.54	122.07
4	d	201	A2G	O3-C3-C2	-3.00	102.96	109.37
4	c	201	A2G	C3-C4-C5	-2.88	105.10	110.23
4	h	201	A2G	C3-C4-C5	-2.83	105.19	110.23
4	a	201	A2G	C8-C7-N2	-2.80	110.73	116.10
4	c	201	A2G	O-C5-C4	-2.73	105.61	110.13
4	h	201	A2G	O-C5-C4	-2.55	105.91	110.13
4	a	201	A2G	O6-C6-C5	-2.39	103.34	111.30
4	g	201	A2G	C3-C4-C5	-2.34	106.05	110.23
4	f	201	A2G	C4-C3-C2	-2.23	107.87	111.34
4	i	201	A2G	C4-C3-C2	-2.20	107.92	111.34
4	g	201	A2G	O-C5-C4	-2.12	106.62	110.13
4	b	201	A2G	C2-N2-C7	-2.09	120.38	123.11
4	a	201	A2G	O4-C4-C5	-2.06	103.81	109.23
4	f	201	A2G	O-C5-C4	-2.05	106.74	110.13
4	i	201	A2G	C3-C4-C5	-2.05	106.58	110.23
4	c	201	A2G	O3-C3-C4	2.01	114.90	110.36
4	j	201	A2G	O7-C7-N2	2.03	125.98	121.84
4	h	201	A2G	O4-C4-C3	2.08	115.05	110.36
4	g	201	A2G	O-C5-C6	2.23	112.12	107.34
4	h	201	A2G	C6-C5-C4	2.45	119.12	112.99
4	a	201	A2G	O4-C4-C3	2.66	116.36	110.36
4	e	201	A2G	O-C5-C6	2.68	113.07	107.34
4	d	201	A2G	O7-C7-N2	2.70	127.35	121.84
4	i	201	A2G	C1-O-C5	2.72	116.15	112.14
4	i	201	A2G	O-C5-C6	2.88	113.52	107.34
4	f	201	A2G	C1-O-C5	3.25	116.92	112.14
4	h	201	A2G	O3-C3-C4	3.28	117.75	110.36
4	b	201	A2G	O-C5-C6	3.34	114.49	107.34
4	f	201	A2G	O3-C3-C4	3.82	118.96	110.36
4	a	201	A2G	O7-C7-C8	3.92	129.29	122.07
4	e	201	A2G	C1-O-C5	4.82	119.23	112.14
4	h	201	A2G	C1-O-C5	4.90	119.35	112.14
4	j	201	A2G	C1-O-C5	5.98	120.93	112.14

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	a	201	A2G	C1-O-C5	8.77	125.04	112.14

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 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	229/242 (94%)	-0.37	0  100  100	30, 41, 56, 76	0
1	B	229/242 (94%)	-0.36	0  100  100	30, 41, 56, 73	0
1	C	229/242 (94%)	-0.10	1 (0%)  93  92	42, 58, 76, 89	0
1	D	229/242 (94%)	-0.26	2 (0%)  85  82	31, 43, 61, 78	0
1	E	229/242 (94%)	-0.04	1 (0%)  93  92	46, 65, 84, 96	0
1	F	229/242 (94%)	-0.26	1 (0%)  93  92	34, 48, 68, 82	0
1	G	229/242 (94%)	0.15	4 (1%)  73  68	54, 72, 95, 108	0
1	H	229/242 (94%)	0.14	6 (2%)  59  53	45, 61, 90, 101	0
1	I	229/242 (94%)	0.25	5 (2%)  65  59	54, 72, 96, 110	0
1	J	229/242 (94%)	0.38	7 (3%)  52  46	61, 76, 98, 110	0
2	a	5/6 (83%)	-0.07	0  100  100	41, 41, 44, 49	0
2	b	5/6 (83%)	0.24	0  100  100	46, 47, 49, 56	0
2	c	5/6 (83%)	0.24	1 (20%)  1  1	62, 66, 70, 75	0
2	d	5/6 (83%)	0.16	0  100  100	39, 39, 41, 46	0
2	e	5/6 (83%)	0.85	1 (20%)  1  1	67, 72, 77, 84	0
2	f	5/6 (83%)	-0.11	0  100  100	43, 43, 46, 50	0
2	g	5/6 (83%)	0.15	0  100  100	67, 68, 70, 72	0
2	h	5/6 (83%)	0.30	0  100  100	57, 58, 60, 61	0
2	i	5/6 (83%)	0.30	1 (20%)  1  1	60, 61, 62, 62	0
2	j	5/6 (83%)	0.43	1 (20%)  1  1	65, 66, 69, 69	0
All	All	2340/2480 (94%)	-0.04	31 (1%)  79  75	30, 58, 89, 110	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	e	105	ALA	4.9
1	J	158	ARG	3.5
2	j	105	ALA	3.5
1	I	229	ASN	3.2
1	H	10	PHE	3.0
1	J	29	LEU	3.0
1	G	51	SER	2.9
1	C	104	ASN	2.8
2	c	105	ALA	2.6
1	J	87	PRO	2.6
1	H	70	ARG	2.5
1	H	11	GLN	2.5
2	i	105	ALA	2.5
1	I	202	VAL	2.5
1	H	158	ARG	2.4
1	H	27	GLU	2.4
1	J	25	ARG	2.4
1	J	57	ARG	2.3
1	G	12	SER	2.3
1	H	57	ARG	2.3
1	G	128	LYS	2.3
1	D	182	ASP	2.2
1	I	87	PRO	2.2
1	F	57	ARG	2.2
1	I	36	SER	2.2
1	E	110	SER	2.2
1	D	229	ASN	2.1
1	G	195	ALA	2.1
1	I	54	PHE	2.1
1	J	50	TYR	2.0
1	J	1	SER	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	A2G	b	201	14/15	0.95	0.18	1.38	38,40,42,44	0
4	A2G	a	201	14/15	0.95	0.17	1.04	35,37,38,38	0
4	A2G	d	201	14/15	0.98	0.16	0.08	32,34,35,36	0
4	A2G	e	201	14/15	0.95	0.17	-0.01	63,67,68,68	0
4	A2G	c	201	14/15	0.97	0.16	-0.21	56,59,61,62	0
4	A2G	f	201	14/15	0.98	0.13	-0.27	37,39,40,41	0
4	A2G	i	201	14/15	0.95	0.14	-0.43	58,60,63,65	0
4	A2G	g	201	14/15	0.97	0.14	-0.59	63,65,66,67	0
4	A2G	h	201	14/15	0.97	0.14	-0.61	52,55,60,61	0
3	CA	H	301	1/1	0.97	0.11	-0.75	49,49,49,49	0
3	CA	C	301	1/1	0.99	0.14	-0.81	47,47,47,47	0
4	A2G	j	201	14/15	0.96	0.14	-0.91	63,65,67,68	0
3	CA	F	302	1/1	0.99	0.09	-1.13	35,35,35,35	0
3	CA	D	302	1/1	0.99	0.10	-1.29	31,31,31,31	0
3	CA	F	301	1/1	0.99	0.08	-1.59	36,36,36,36	0
3	CA	J	301	1/1	0.98	0.08	-1.70	59,59,59,59	0
3	CA	B	301	1/1	0.99	0.09	-1.80	33,33,33,33	0
3	CA	J	302	1/1	0.99	0.04	-1.97	61,61,61,61	0
3	CA	I	301	1/1	0.97	0.12	-2.02	52,52,52,52	0
3	CA	A	302	1/1	0.97	0.08	-2.40	36,36,36,36	0
3	CA	E	301	1/1	0.98	0.07	-2.60	54,54,54,54	0
3	CA	A	301	1/1	0.99	0.09	-2.78	32,32,32,32	0
3	CA	G	301	1/1	0.96	0.04	-2.93	60,60,60,60	0
3	CA	G	302	1/1	0.98	0.08	-2.97	59,59,59,59	0
3	CA	C	302	1/1	0.97	0.08	-3.00	54,54,54,54	0
3	CA	H	302	1/1	0.99	0.09	-3.02	52,52,52,52	0
3	CA	E	302	1/1	0.98	0.06	-3.07	62,62,62,62	0
3	CA	B	302	1/1	0.99	0.09	-3.86	36,36,36,36	0
3	CA	I	302	1/1	0.99	0.08	-4.21	55,55,55,55	0
3	CA	D	301	1/1	1.00	0.09	-4.87	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.