



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:41 AM GMT

PDB ID : 3FHZ  
Title : Crystal structure of the arginine repressor from Mycobacterium tuberculosis bound with its DNA operator and co-repressor, L-arginine  
Authors : Cherney, L.T.; Cherney, M.M.; Garen, C.R.; James, M.N.G.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2008-12-10  
Resolution : 3.27 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

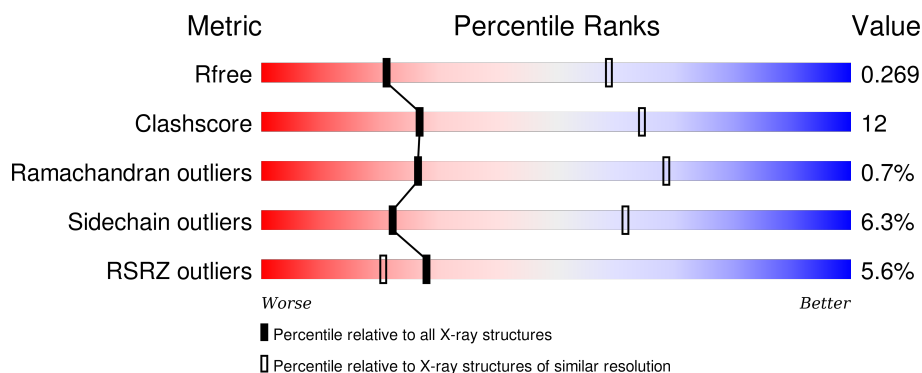
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1756 (3.36-3.20)
Clashscore	102246	1941 (3.36-3.20)
Ramachandran outliers	100387	1905 (3.36-3.20)
Sidechain outliers	100360	1903 (3.36-3.20)
RSRZ outliers	91569	1764 (3.36-3.20)

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	170	<div> <div>5%</div> <div>68% 19% 9%</div> </div>
1	B	170	<div> <div>5%</div> <div>61% 28% 5% 5%</div> </div>
1	C	170	<div> <div>2%</div> <div>61% 27% 6% 6%</div> </div>
1	D	170	<div> <div>5%</div> <div>62% 28% 8% .</div> </div>
1	E	170	<div> <div>10%</div> <div>72% 16% . 9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	170	
2	G	20	
2	I	20	
2	K	20	
3	H	20	
3	J	20	
3	L	20	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ARG	A	302	-	-	-	X
4	ARG	B	301	-	-	-	X
4	ARG	C	300	-	-	-	X
4	ARG	D	200	-	-	-	X
4	ARG	F	200	-	-	-	X
5	ACT	A	400	-	-	-	X
6	GOL	D	500	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9454 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 Arginine repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1117	685	207	223	2			
1	B	161	Total	C	N	O	S	0	0	0
			1154	708	213	231	2			
1	C	160	Total	C	N	O	S	0	0	0
			1149	705	212	230	2			
1	D	166	Total	C	N	O	S	0	0	0
			1187	730	219	236	2			
1	E	155	Total	C	N	O	S	0	0	0
			1117	685	207	223	2			
1	F	155	Total	C	N	O	S	0	0	0
			1117	685	207	223	2			

- Molecule 2 is a DNA chain called 5'-D(\*TP\*GP\*TP\*TP\*GP\*CP\*AP\*TP\*AP\*AP\*CP\*GP\*AP\*TP\*GP\*CP\*AP\*AP\*AP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	20	Total	C	N	O	P	0	0	0
			410	197	79	115	19			
2	I	20	Total	C	N	O	P	0	0	0
			410	197	79	115	19			
2	K	20	Total	C	N	O	P	0	0	0
			410	197	79	115	19			

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

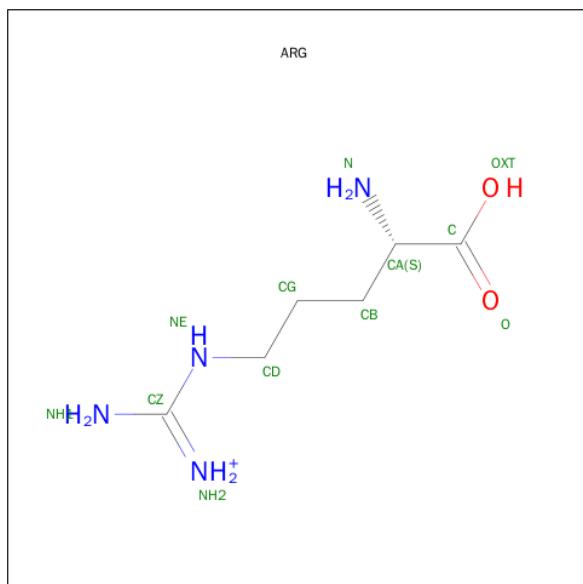
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	20	Total	C	N	O	P	0	0	0
			404	196	68	121	19			
3	J	20	Total	C	N	O	P	0	0	0
			404	196	68	121	19			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	20	Total	C	N	O	P	0	0	0
			404	196	68	121	19			

- Molecule 4 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	6	4	2		
4	B	1	Total	C	N	O	0	0
			12	6	4	2		
4	C	1	Total	C	N	O	0	0
			12	6	4	2		
4	D	1	Total	C	N	O	0	0
			12	6	4	2		
4	E	1	Total	C	N	O	0	0
			12	6	4	2		
4	F	1	Total	C	N	O	0	0
			12	6	4	2		
4	A	1	Total	C	N		0	0
			4	1	3			
4	B	1	Total	C	N		0	0
			4	1	3			
4	C	1	Total	C	N		0	0
			4	1	3			

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



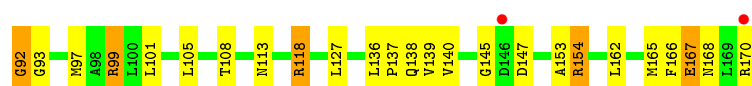
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

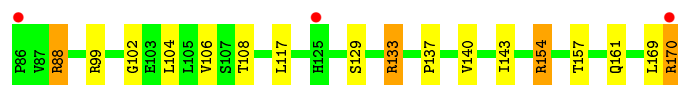
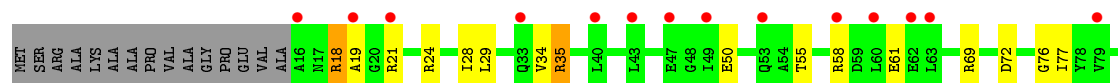
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total 6	O 6	0	0
7	B	15	Total 15	O 15	0	0
7	C	12	Total 12	O 12	0	0
7	D	16	Total 16	O 16	0	0
7	E	5	Total 5	O 5	0	0
7	F	12	Total 12	O 12	0	0
7	I	1	Total 1	O 1	0	0
7	L	6	Total 6	O 6	0	0



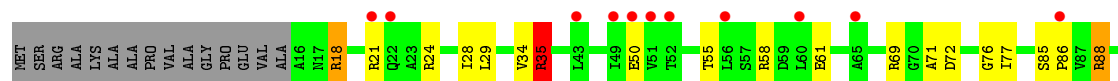




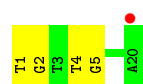
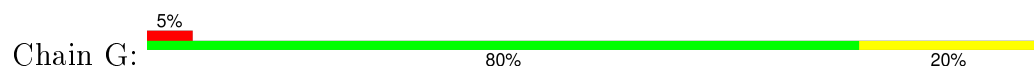
- Molecule 1: Arginine repressor



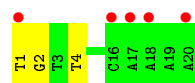
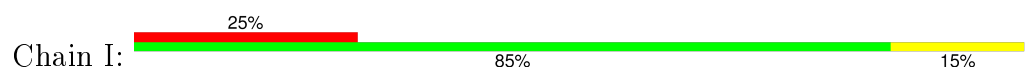
- Molecule 1: Arginine repressor



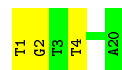
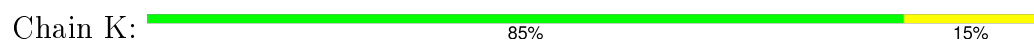
- Molecule 2: 5'-D(\*TP\*GP\*TP\*TP\*GP\*CP\*AP\*TP\*AP\*AP\*CP\*GP\*AP\*TP\*GP\*CP\*AP\*A P\*AP\*A)-3'



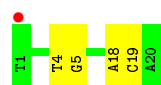
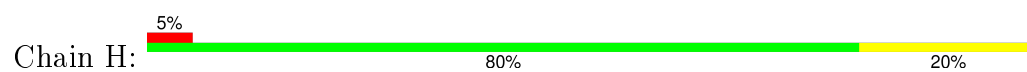
- Molecule 2: 5'-D(\*TP\*GP\*TP\*TP\*GP\*CP\*AP\*TP\*AP\*AP\*CP\*GP\*AP\*TP\*GP\*CP\*AP\*A P\*AP\*A)-3'



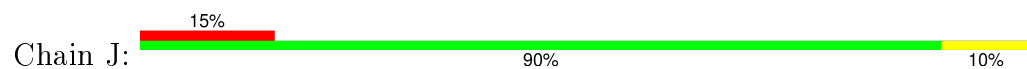
- Molecule 2: 5'-D(\*TP\*GP\*TP\*TP\*GP\*CP\*AP\*TP\*AP\*AP\*CP\*GP\*AP\*TP\*GP\*CP\*AP\*A P\*AP\*A)-3'



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



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.29Å 152.65Å 163.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.34 – 3.27 44.34 – 3.27	Depositor EDS
% Data completeness (in resolution range)	97.4 (44.34-3.27) 97.4 (44.34-3.27)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 3.25Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.231 , 0.276 0.217 , 0.269	Depositor DCC
$R_{free}$ test set	1244 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	96.9	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 66.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 24617 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9454	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, ACT

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	0.24	0/1126	1.04	13/1528 (0.9%)
1	B	0.24	0/1164	0.98	13/1581 (0.8%)
1	C	0.26	0/1159	1.29	16/1574 (1.0%)
1	D	0.24	0/1198	0.96	13/1628 (0.8%)
1	E	0.28	0/1126	1.39	16/1528 (1.0%)
1	F	0.23	0/1126	1.02	13/1528 (0.9%)
2	G	0.43	0/461	0.96	0/710
2	I	0.42	0/461	0.94	0/710
2	K	0.42	0/461	0.93	0/710
3	H	0.42	0/451	1.04	0/694
3	J	0.42	0/451	1.04	0/694
3	L	0.42	0/451	1.04	0/694
All	All	0.31	0/9635	1.09	84/13579 (0.6%)

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	35	ARG	NE-CZ-NH1	-18.77	110.92	120.30
1	E	35	ARG	NE-CZ-NH2	17.84	129.22	120.30
1	E	99	ARG	NE-CZ-NH1	-17.23	111.68	120.30
1	C	170	ARG	NE-CZ-NH2	-16.96	111.82	120.30
1	A	21	ARG	NE-CZ-NH2	-16.66	111.97	120.30
1	D	118	ARG	NE-CZ-NH2	-16.20	112.20	120.30
1	E	154	ARG	NE-CZ-NH2	-16.17	112.21	120.30
1	C	170	ARG	NE-CZ-NH1	16.14	128.37	120.30
1	A	21	ARG	NE-CZ-NH1	16.10	128.35	120.30
1	F	133	ARG	NE-CZ-NH1	-16.06	112.27	120.30
1	B	21	ARG	NE-CZ-NH1	-16.01	112.29	120.30
1	C	154	ARG	NE-CZ-NH1	-15.92	112.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	99	ARG	NE-CZ-NH2	15.83	128.22	120.30
1	F	133	ARG	NE-CZ-NH2	15.73	128.17	120.30
1	B	21	ARG	NE-CZ-NH2	15.62	128.11	120.30
1	E	154	ARG	NE-CZ-NH1	15.30	127.95	120.30
1	C	154	ARG	NE-CZ-NH2	15.03	127.81	120.30
1	D	118	ARG	NE-CZ-NH1	14.75	127.67	120.30
1	C	99	ARG	NE-CZ-NH2	-14.71	112.94	120.30
1	C	99	ARG	NE-CZ-NH1	14.20	127.40	120.30
1	E	170	ARG	NE-CZ-NH1	-14.12	113.24	120.30
1	C	18	ARG	NE-CZ-NH1	-14.04	113.28	120.30
1	E	170	ARG	NE-CZ-NH2	13.63	127.12	120.30
1	C	18	ARG	NE-CZ-NH2	13.54	127.07	120.30
1	F	35	ARG	NE-CZ-NH2	-10.37	115.11	120.30
1	A	35	ARG	NE-CZ-NH2	-10.12	115.24	120.30
1	E	35	ARG	CD-NE-CZ	8.99	136.18	123.60
1	D	170	ARG	NE-CZ-NH1	-8.61	116.00	120.30
1	E	21	ARG	NE-CZ-NH1	-8.58	116.01	120.30
1	A	133	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	A	99	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	B	170	ARG	NE-CZ-NH1	-8.56	116.02	120.30
1	C	118	ARG	NE-CZ-NH1	-8.51	116.05	120.30
1	A	154	ARG	NE-CZ-NH1	-8.44	116.08	120.30
1	F	99	ARG	NE-CZ-NH2	-8.39	116.10	120.30
1	B	118	ARG	NE-CZ-NH1	-8.37	116.12	120.30
1	F	21	ARG	NE-CZ-NH1	-8.36	116.12	120.30
1	E	133	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	E	21	ARG	NE-CZ-NH2	8.30	124.45	120.30
1	F	154	ARG	NE-CZ-NH1	-8.26	116.17	120.30
1	A	99	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	F	99	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	D	170	ARG	NE-CZ-NH2	8.24	124.42	120.30
1	B	154	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	F	21	ARG	NE-CZ-NH2	8.19	124.39	120.30
1	A	21	ARG	CD-NE-CZ	8.14	135.00	123.60
1	B	170	ARG	NE-CZ-NH2	8.13	124.37	120.30
1	D	154	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	C	170	ARG	CD-NE-CZ	8.08	134.91	123.60
1	A	35	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	B	118	ARG	NE-CZ-NH2	8.01	124.31	120.30
1	F	133	ARG	CD-NE-CZ	7.98	134.77	123.60
1	E	133	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	B	99	ARG	NE-CZ-NH1	-7.94	116.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	21	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	C	118	ARG	NE-CZ-NH2	7.91	124.25	120.30
1	F	35	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	C	21	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	A	133	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	E	99	ARG	CD-NE-CZ	7.83	134.56	123.60
1	D	99	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	F	154	ARG	NE-CZ-NH2	7.72	124.16	120.30
1	C	21	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	B	21	ARG	CD-NE-CZ	7.65	134.31	123.60
1	E	154	ARG	CD-NE-CZ	7.62	134.26	123.60
1	C	154	ARG	CD-NE-CZ	7.49	134.08	123.60
1	B	154	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	A	154	ARG	NE-CZ-NH2	7.47	124.03	120.30
1	D	154	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	D	21	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	99	ARG	NE-CZ-NH2	7.35	123.97	120.30
1	F	170	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	D	118	ARG	CD-NE-CZ	7.28	133.79	123.60
1	D	99	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	A	170	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	D	18	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	B	18	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	170	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	F	170	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	D	18	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	C	99	ARG	CD-NE-CZ	6.79	133.11	123.60
1	B	18	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	C	18	ARG	CD-NE-CZ	6.42	132.59	123.60
1	E	170	ARG	CD-NE-CZ	6.18	132.26	123.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1117	0	1138	33	0
1	B	1154	0	1173	46	0
1	C	1149	0	1168	42	0
1	D	1187	0	1212	51	0
1	E	1117	0	1138	28	0
1	F	1117	0	1138	28	0
2	G	410	0	227	8	0
2	I	410	0	227	3	0
2	K	410	0	227	3	0
3	H	404	0	230	4	0
3	J	404	0	230	1	0
3	L	404	0	230	6	0
4	A	16	0	16	1	0
4	B	16	0	16	1	0
4	C	16	0	16	3	0
4	D	12	0	12	0	0
4	E	12	0	12	1	0
4	F	12	0	12	2	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	D	6	0	8	1	0
7	A	6	0	0	0	0
7	B	15	0	0	0	0
7	C	12	0	0	0	0
7	D	16	0	0	0	0
7	E	5	0	0	0	0
7	F	12	0	0	0	0
7	I	1	0	0	0	0
7	L	6	0	0	0	0
All	All	9454	0	8436	215	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 12.

All (215) 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:93:GLY:HA2	1:E:72:ASP:HB3	1.48	0.94
1:A:88:ARG:HG3	1:A:88:ARG:HH11	1.45	0.82
1:C:137:PRO:O	1:C:154:ARG:HD2	1.80	0.82
1:E:88:ARG:HH11	1:E:88:ARG:HG3	1.45	0.80
1:F:88:ARG:HG3	1:F:88:ARG:HH11	1.44	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:GLY:HA2	1:F:72:ASP:HB3	1.67	0.76
1:B:15:ALA:HA	1:E:170:ARG:NH1	2.02	0.74
1:A:72:ASP:HB3	1:D:93:GLY:HA2	1.70	0.74
1:B:35:ARG:CG	1:B:35:ARG:HH11	2.04	0.71
2:G:1:DT:H5'	3:L:20:DA:H1'	1.73	0.70
1:D:35:ARG:HH11	1:D:35:ARG:CG	2.05	0.69
1:B:15:ALA:HA	1:E:170:ARG:CZ	2.24	0.68
1:C:35:ARG:HH11	1:C:35:ARG:CG	2.06	0.68
1:B:97:MET:O	1:B:101:LEU:HB2	1.93	0.68
1:C:97:MET:O	1:C:101:LEU:HB2	1.94	0.68
1:D:97:MET:O	1:D:101:LEU:HB2	1.94	0.67
1:A:118:ARG:HH21	1:B:84:GLY:HA2	1.59	0.66
1:D:101:LEU:HD21	1:D:166:PHE:HD1	1.61	0.66
1:C:101:LEU:HD21	1:C:166:PHE:HD1	1.60	0.65
1:B:101:LEU:HD21	1:B:166:PHE:HD1	1.62	0.65
1:F:140:VAL:HG22	1:F:154:ARG:HB3	1.79	0.64
1:B:35:ARG:HG3	1:B:35:ARG:HH11	1.62	0.64
1:A:55:THR:HG21	3:L:4:DT:C2'	2.28	0.64
1:A:111:SER:HB2	1:B:140:VAL:HG21	1.80	0.63
1:A:18:ARG:HG2	1:A:21:ARG:NH2	2.13	0.63
1:E:55:THR:HG21	3:H:4:DT:C2'	2.29	0.63
1:D:145:GLY:HA3	4:F:200:ARG:OXT	1.98	0.63
1:F:91:SER:HB3	1:F:133:ARG:HD2	1.79	0.62
1:A:140:VAL:HG22	1:A:154:ARG:HB3	1.80	0.62
1:C:170:ARG:HH22	1:D:16:ALA:HB3	1.65	0.62
1:E:140:VAL:HG22	1:E:154:ARG:HB3	1.82	0.62
1:C:55:THR:CG2	2:G:4:DT:H2'	2.30	0.61
1:D:84:GLY:HA2	1:F:118:ARG:HH21	1.65	0.61
1:C:35:ARG:HG3	1:C:35:ARG:HH11	1.66	0.61
1:C:61:GLU:HA	1:E:69:ARG:NH1	2.15	0.60
1:E:18:ARG:C	1:E:18:ARG:HD3	2.22	0.60
1:E:55:THR:HG21	3:H:4:DT:H2''	1.83	0.60
1:B:138:GLN:HE21	1:B:165:MET:HE1	1.66	0.60
1:D:35:ARG:HH11	1:D:35:ARG:HG3	1.66	0.59
1:D:138:GLN:HE21	1:D:165:MET:HE1	1.67	0.59
1:C:138:GLN:HE21	1:C:165:MET:HE1	1.67	0.59
1:C:52:THR:HG21	2:G:5:DG:H3'	1.84	0.58
1:D:138:GLN:HE21	1:D:165:MET:CE	2.17	0.57
1:C:138:GLN:HE21	1:C:165:MET:CE	2.18	0.57
1:A:118:ARG:HH21	1:B:84:GLY:CA	2.17	0.57
1:B:138:GLN:HE21	1:B:165:MET:CE	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ARG:HE	1:B:84:GLY:HA2	1.70	0.57
1:E:55:THR:HA	1:E:58:ARG:HD2	1.88	0.56
1:A:18:ARG:HG2	1:A:21:ARG:HH22	1.69	0.55
1:A:55:THR:HA	1:A:58:ARG:HD2	1.89	0.55
1:A:55:THR:HG21	3:L:4:DT:H2'	1.87	0.55
1:F:55:THR:HA	1:F:58:ARG:HD2	1.88	0.54
1:D:35:ARG:NH1	1:D:35:ARG:CG	2.67	0.54
1:F:88:ARG:CG	1:F:88:ARG:HH11	2.17	0.54
1:C:57:SER:O	1:C:61:GLU:HB3	2.08	0.54
1:B:57:SER:O	1:B:61:GLU:HB3	2.08	0.54
1:A:170:ARG:HG2	1:A:170:ARG:O	2.08	0.54
2:G:1:DT:C5'	3:L:20:DA:H1'	2.38	0.53
1:D:14:VAL:HG12	1:D:15:ALA:H	1.74	0.53
1:E:102:GLY:HA2	1:E:170:ARG:HG3	1.90	0.53
1:D:57:SER:O	1:D:61:GLU:HB3	2.08	0.53
1:B:64:GLY:HA3	1:F:71:ALA:HA	1.91	0.53
1:B:14:VAL:HG12	1:B:15:ALA:H	1.72	0.53
1:C:14:VAL:HG12	1:C:15:ALA:H	1.74	0.53
1:A:69:ARG:NH1	1:D:61:GLU:HA	2.23	0.52
1:A:88:ARG:CG	1:A:88:ARG:HH11	2.17	0.52
1:C:84:GLY:C	1:C:86:PRO:HD3	2.30	0.52
1:B:84:GLY:C	1:B:86:PRO:HD3	2.31	0.52
1:E:88:ARG:HH11	1:E:88:ARG:CG	2.17	0.52
1:F:88:ARG:HG3	1:F:88:ARG:NH1	2.21	0.52
1:D:69:ARG:HA	1:D:76:GLY:HA3	1.92	0.52
1:D:56:LEU:O	1:D:60:LEU:HG	2.10	0.52
1:D:84:GLY:C	1:D:86:PRO:HD3	2.31	0.51
1:A:150:LEU:HD22	1:B:143:ILE:HG21	1.92	0.51
1:C:55:THR:HG23	2:G:4:DT:H2'	1.91	0.51
1:F:170:ARG:O	1:F:170:ARG:HG2	2.09	0.51
4:A:200:ARG:N	1:C:148:THR:HG1	2.08	0.51
1:B:137:PRO:HG2	1:B:138:GLN:OE1	2.09	0.51
1:F:58:ARG:O	1:F:61:GLU:HB3	2.10	0.51
1:A:76:GLY:C	1:A:77:ILE:HD12	2.31	0.51
1:C:56:LEU:O	1:C:60:LEU:HG	2.11	0.51
1:B:56:LEU:O	1:B:60:LEU:HG	2.10	0.51
1:C:69:ARG:HA	1:C:76:GLY:HA3	1.93	0.51
1:A:58:ARG:O	1:A:61:GLU:HB3	2.10	0.51
1:D:8:PRO:HG3	1:D:13:GLU:HG3	1.93	0.51
1:A:71:ALA:HA	1:D:64:GLY:HA3	1.91	0.51
1:C:137:PRO:HG2	1:C:138:GLN:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ARG:HG3	1:A:88:ARG:NH1	2.22	0.50
1:E:58:ARG:O	1:E:61:GLU:HB3	2.11	0.50
1:B:69:ARG:HA	1:B:76:GLY:HA3	1.93	0.50
1:C:93:GLY:HA2	1:E:72:ASP:CB	2.31	0.50
1:B:35:ARG:NH1	1:B:35:ARG:CG	2.66	0.49
1:D:137:PRO:HG2	1:D:138:GLN:OE1	2.11	0.49
1:E:76:GLY:C	1:E:77:ILE:HD12	2.33	0.49
1:D:6:ALA:HB1	1:D:12:PRO:O	2.13	0.48
4:E:200:ARG:O	1:F:145:GLY:HA3	2.13	0.48
1:F:76:GLY:C	1:F:77:ILE:HD12	2.34	0.48
1:E:18:ARG:HD3	1:E:19:ALA:N	2.28	0.48
1:E:88:ARG:NH1	1:E:88:ARG:HG3	2.22	0.48
1:C:35:ARG:NH1	1:C:35:ARG:CG	2.68	0.48
1:C:68:LEU:HD12	1:C:69:ARG:N	2.29	0.48
1:B:68:LEU:HD12	1:B:69:ARG:N	2.29	0.48
1:F:24:ARG:O	1:F:28:ILE:HG13	2.14	0.48
1:B:21:ARG:O	1:B:25:ILE:HG13	2.14	0.47
4:C:200:ARG:HD2	1:F:129:SER:CB	2.44	0.47
1:D:18:ARG:HD3	2:K:4:DT:OP2	2.14	0.47
3:H:18:DA:H1'	3:H:19:DC:H5'	1.96	0.47
1:C:11:GLY:HA2	1:C:12:PRO:C	2.34	0.47
3:L:18:DA:H1'	3:L:19:DC:H5'	1.96	0.47
1:D:5:LYS:O	1:D:5:LYS:HD2	2.14	0.47
1:E:24:ARG:O	1:E:28:ILE:HG13	2.14	0.47
1:D:5:LYS:O	1:D:6:ALA:HB2	2.14	0.47
3:J:18:DA:H1'	3:J:19:DC:H5'	1.96	0.47
1:A:24:ARG:O	1:A:28:ILE:HG13	2.14	0.47
1:A:52:THR:HG21	3:L:5:DG:H3'	1.97	0.47
1:D:68:LEU:HD12	1:D:69:ARG:N	2.30	0.47
1:B:167:GLU:OE1	1:B:167:GLU:HA	2.16	0.46
1:D:21:ARG:O	1:D:25:ILE:HG13	2.14	0.46
1:B:68:LEU:HD12	1:B:69:ARG:H	1.81	0.46
1:E:137:PRO:O	1:E:154:ARG:HD2	2.16	0.46
1:D:153:ALA:HB2	1:D:162:LEU:CD1	2.45	0.46
1:B:61:GLU:HA	1:F:69:ARG:NH1	2.31	0.46
1:A:129:SER:O	1:A:133:ARG:HG2	2.16	0.46
1:C:21:ARG:O	1:C:25:ILE:HG13	2.16	0.45
1:A:146:ASP:OD1	4:C:200:ARG:NH1	2.49	0.45
1:F:85:SER:HA	1:F:86:PRO:HD3	1.83	0.45
1:B:153:ALA:HB2	1:B:162:LEU:CD1	2.46	0.45
1:C:153:ALA:HB2	1:C:162:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:GLU:OE1	1:D:167:GLU:HA	2.16	0.45
1:E:129:SER:O	1:E:133:ARG:HG2	2.16	0.45
1:B:14:VAL:HG12	1:B:15:ALA:N	2.31	0.45
1:C:68:LEU:HD12	1:C:69:ARG:H	1.81	0.45
1:C:167:GLU:HA	1:C:167:GLU:OE1	2.16	0.45
1:D:68:LEU:HD12	1:D:69:ARG:H	1.82	0.45
1:B:55:THR:CG2	2:I:4:DT:H2'	2.46	0.45
1:C:55:THR:HG21	2:G:4:DT:H2'	1.98	0.45
1:A:85:SER:HA	1:A:86:PRO:HD3	1.83	0.45
1:D:140:VAL:HG21	1:F:111:SER:HB2	1.99	0.44
1:D:136:LEU:O	1:D:139:VAL:HG22	2.18	0.44
1:F:29:LEU:HD23	1:F:34:VAL:HG21	2.00	0.44
1:B:91:SER:O	1:B:92:GLY:O	2.36	0.44
2:K:1:DT:H2''	2:K:2:DG:C8	2.52	0.44
1:B:20:GLY:HA2	1:E:106:VAL:HG13	2.00	0.44
1:D:118:ARG:HD3	1:D:147:ASP:O	2.16	0.44
1:B:136:LEU:O	1:B:139:VAL:HG22	2.17	0.44
1:B:105:LEU:HD21	1:B:108:THR:HG23	2.00	0.44
1:B:21:ARG:HD2	1:B:59:ASP:OD1	2.18	0.44
1:D:21:ARG:HD3	1:D:51:VAL:HG11	2.00	0.44
1:D:105:LEU:HD21	1:D:108:THR:HG23	2.00	0.44
1:C:136:LEU:O	1:C:139:VAL:HG22	2.17	0.43
2:G:1:DT:H2''	2:G:2:DG:C8	2.53	0.43
1:D:14:VAL:HG12	1:D:15:ALA:N	2.33	0.43
1:B:73:GLY:O	1:B:74:GLY:C	2.56	0.43
1:D:73:GLY:O	1:D:74:GLY:C	2.57	0.43
1:B:140:VAL:HG22	1:B:154:ARG:HB3	1.99	0.43
1:D:40:LEU:HD23	1:D:56:LEU:HD13	1.99	0.43
1:C:73:GLY:O	1:C:74:GLY:C	2.57	0.43
1:B:101:LEU:HA	1:B:101:LEU:HD12	1.84	0.43
1:D:54:ALA:O	1:D:58:ARG:HG3	2.19	0.43
1:E:88:ARG:NH1	1:E:88:ARG:CG	2.78	0.43
1:D:140:VAL:HG22	1:D:154:ARG:HB3	2.00	0.43
1:A:88:ARG:NH1	1:A:88:ARG:CG	2.78	0.43
1:B:40:LEU:HD23	1:B:56:LEU:HD13	1.99	0.43
2:I:1:DT:H2''	2:I:2:DG:C8	2.52	0.43
1:A:29:LEU:HD23	1:A:34:VAL:HG21	2.01	0.43
1:D:101:LEU:HD12	1:D:101:LEU:HA	1.83	0.43
1:A:145:GLY:HA3	4:B:200:ARG:O	2.18	0.43
1:C:21:ARG:HD3	1:C:51:VAL:HG11	2.00	0.43
1:E:170:ARG:O	1:E:170:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ALA:O	1:C:58:ARG:HG3	2.19	0.42
1:C:91:SER:O	1:C:92:GLY:O	2.37	0.42
1:E:29:LEU:HD23	1:E:34:VAL:HG21	2.00	0.42
1:D:35:ARG:NH1	1:D:35:ARG:HG2	2.35	0.42
1:C:14:VAL:HG12	1:C:15:ALA:N	2.33	0.42
2:K:1:DT:H2"	2:K:2:DG:H8	1.84	0.42
1:B:54:ALA:O	1:B:58:ARG:HG3	2.19	0.42
1:F:88:ARG:CG	1:F:88:ARG:NH1	2.77	0.42
2:G:1:DT:H2"	2:G:2:DG:H8	1.85	0.42
1:B:22:GLN:O	1:B:26:VAL:HG12	2.19	0.42
1:C:61:GLU:HG3	1:C:62:GLU:N	2.34	0.42
1:A:167:GLU:OE2	1:A:170:ARG:NH2	2.53	0.42
1:D:61:GLU:HG3	1:D:62:GLU:N	2.35	0.42
1:F:35:ARG:HE	1:F:35:ARG:HB3	1.64	0.42
1:B:61:GLU:HG3	1:B:62:GLU:N	2.35	0.42
1:B:60:LEU:HA	1:B:63:LEU:HB2	2.02	0.42
1:B:45:ALA:C	1:B:47:GLU:H	2.23	0.42
1:F:167:GLU:OE2	1:F:170:ARG:NH2	2.53	0.41
1:D:113:ASN:ND2	1:F:111:SER:O	2.52	0.41
1:C:90:VAL:HG12	1:C:91:SER:H	1.85	0.41
1:A:108:THR:HG22	1:A:117:LEU:CD2	2.50	0.41
1:E:108:THR:HG22	1:E:117:LEU:CD2	2.50	0.41
1:D:91:SER:O	1:D:92:GLY:O	2.37	0.41
1:C:22:GLN:O	1:C:26:VAL:HG12	2.19	0.41
1:D:60:LEU:HA	1:D:63:LEU:HB2	2.03	0.41
1:C:40:LEU:HD23	1:C:56:LEU:HD13	2.01	0.41
1:E:143:ILE:HA	4:F:200:ARG:N	2.35	0.41
1:C:105:LEU:HD21	1:C:108:THR:HG23	2.01	0.41
1:F:108:THR:HG22	1:F:117:LEU:CD2	2.51	0.41
1:C:45:ALA:C	1:C:47:GLU:H	2.24	0.41
1:D:99:ARG:NH2	6:D:500:GOL:O1	2.54	0.41
1:A:65:ALA:O	1:D:69:ARG:NH1	2.52	0.41
1:F:157:THR:HA	1:F:161:GLN:OE1	2.20	0.41
1:E:157:THR:HA	1:E:161:GLN:OE1	2.20	0.41
1:D:45:ALA:C	1:D:47:GLU:H	2.23	0.41
1:C:140:VAL:HG22	1:C:154:ARG:HB3	2.02	0.41
1:D:84:GLY:CA	1:F:118:ARG:HH21	2.31	0.41
1:D:56:LEU:HD23	1:D:56:LEU:HA	1.92	0.40
1:B:80:VAL:HA	1:B:81:PRO:HD2	1.92	0.40
1:A:118:ARG:NH2	1:B:84:GLY:HA2	2.30	0.40
4:C:200:ARG:HD2	1:F:129:SER:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1:DT:H2"	2:I:2:DG:H8	1.84	0.40
1:E:55:THR:HG21	3:H:5:DG:OP2	2.21	0.40
1:F:18:ARG:HB3	1:F:18:ARG:CZ	2.51	0.40
1:D:90:VAL:HG12	1:D:91:SER:H	1.85	0.40
1:A:45:ALA:C	1:A:47:GLU:H	2.25	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	153/170 (90%)	141 (92%)	12 (8%)	0	100	100
1	B	159/170 (94%)	138 (87%)	19 (12%)	2 (1%)	15	55
1	C	158/170 (93%)	137 (87%)	19 (12%)	2 (1%)	15	55
1	D	164/170 (96%)	140 (85%)	21 (13%)	3 (2%)	11	49
1	E	153/170 (90%)	141 (92%)	12 (8%)	0	100	100
1	F	153/170 (90%)	141 (92%)	12 (8%)	0	100	100
All	All	940/1020 (92%)	838 (89%)	95 (10%)	7 (1%)	26	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	74	GLY
1	C	74	GLY
1	D	74	GLY
1	B	92	GLY
1	C	92	GLY
1	D	6	ALA
1	D	92	GLY

### 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	113/122 (93%)	107 (95%)	6 (5%)	28	68
1	B	116/122 (95%)	108 (93%)	8 (7%)	19	58
1	C	116/122 (95%)	108 (93%)	8 (7%)	19	58
1	D	119/122 (98%)	110 (92%)	9 (8%)	16	53
1	E	113/122 (93%)	107 (95%)	6 (5%)	28	68
1	F	113/122 (93%)	106 (94%)	7 (6%)	23	62
All	All	690/732 (94%)	646 (94%)	44 (6%)	22	61

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	35	ARG
1	A	50	GLU
1	A	88	ARG
1	A	104	LEU
1	A	169	LEU
1	B	35	ARG
1	B	55	THR
1	B	60	LEU
1	B	61	GLU
1	B	75	THR
1	B	127	LEU
1	B	167	GLU
1	B	168	ASN
1	C	35	ARG
1	C	55	THR
1	C	60	LEU
1	C	61	GLU
1	C	75	THR
1	C	127	LEU
1	C	167	GLU
1	C	168	ASN

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Mol	Chain	Res	Type
1	D	5	LYS
1	D	35	ARG
1	D	55	THR
1	D	60	LEU
1	D	61	GLU
1	D	75	THR
1	D	127	LEU
1	D	167	GLU
1	D	168	ASN
1	E	18	ARG
1	E	35	ARG
1	E	50	GLU
1	E	88	ARG
1	E	104	LEU
1	E	169	LEU
1	F	18	ARG
1	F	35	ARG
1	F	50	GLU
1	F	88	ARG
1	F	104	LEU
1	F	133	ARG
1	F	169	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	E	168	ASN
1	F	168	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 ⓘ

12 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	$\# Z  > 2$
4	ARG	A	200	-	5,11,11	0.34	0	3,13,13	0.19	0
4	ARG	A	302	-	0,3,11	0.00	-	0,3,13	0.00	-
5	ACT	A	400	-	1,3,3	1.24	0	0,3,3	0.00	-
4	ARG	B	200	-	5,11,11	0.31	0	3,13,13	0.19	0
4	ARG	B	301	-	0,3,11	0.00	-	0,3,13	0.00	-
5	ACT	B	401	-	1,3,3	1.31	0	0,3,3	0.00	-
4	ARG	C	200	-	5,11,11	0.34	0	3,13,13	0.76	0
4	ARG	C	300	-	0,3,11	0.00	-	0,3,13	0.00	-
4	ARG	D	200	-	5,11,11	0.35	0	3,13,13	0.17	0
6	GOL	D	500	-	5,5,5	0.26	0	5,5,5	0.26	0
4	ARG	E	200	-	5,11,11	0.36	0	3,13,13	0.29	0
4	ARG	F	200	-	5,11,11	0.38	0	3,13,13	0.29	0

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	ARG	A	200	-	-	0/5/11/11	0/0/0/0
4	ARG	A	302	-	-	0/0/0/11	0/0/0/0
5	ACT	A	400	-	-	0/0/0/0	0/0/0/0
4	ARG	B	200	-	-	0/5/11/11	0/0/0/0
4	ARG	B	301	-	-	0/0/0/11	0/0/0/0
5	ACT	B	401	-	-	0/0/0/0	0/0/0/0
4	ARG	C	200	-	-	0/5/11/11	0/0/0/0
4	ARG	C	300	-	-	0/0/0/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ARG	D	200	-	-	0/5/11/11	0/0/0/0
6	GOL	D	500	-	-	0/4/4/4	0/0/0/0
4	ARG	E	200	-	-	0/5/11/11	0/0/0/0
4	ARG	F	200	-	-	0/5/11/11	0/0/0/0

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.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	200	ARG	1	0
4	B	200	ARG	1	0
4	C	200	ARG	3	0
6	D	500	GOL	1	0
4	E	200	ARG	1	0
4	F	200	ARG	2	0

## 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	155/170 (91%)	0.20	2 (1%) 79 72	62, 103, 151, 184	0
1	B	161/170 (94%)	0.34	8 (4%) 32 25	62, 96, 148, 196	0
1	C	160/170 (94%)	0.31	4 (2%) 61 52	64, 98, 149, 204	0
1	D	166/170 (97%)	0.27	8 (4%) 34 27	64, 95, 164, 197	0
1	E	155/170 (91%)	0.78	17 (10%) 7 5	69, 111, 164, 194	0
1	F	155/170 (91%)	0.35	11 (7%) 19 14	65, 109, 164, 183	0
2	G	20/20 (100%)	0.43	1 (5%) 32 25	124, 160, 201, 207	0
2	I	20/20 (100%)	0.96	5 (25%) 1 1	127, 166, 198, 208	0
2	K	20/20 (100%)	-0.34	0 100 100	118, 150, 190, 199	0
3	H	20/20 (100%)	0.54	1 (5%) 32 25	117, 162, 177, 190	0
3	J	20/20 (100%)	1.01	3 (15%) 3 2	123, 166, 191, 192	0
3	L	20/20 (100%)	-0.36	0 100 100	106, 152, 178, 178	0
All	All	1072/1140 (94%)	0.37	60 (5%) 28 21	62, 106, 173, 208	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	43	LEU	6.0
3	J	20	DA	5.0
1	D	6	ALA	4.6
1	E	170	ARG	4.0
1	E	49	ILE	4.0
1	F	51	VAL	3.9
1	F	50	GLU	3.9
2	I	17	DA	3.7
1	D	7	ALA	3.7
1	C	77	ILE	3.7
1	B	34	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
2	I	16	DC	3.6
1	A	49	ILE	3.5
1	F	52	THR	3.4
1	F	86	PRO	3.4
1	E	79	VAL	3.4
1	B	71	ALA	3.4
1	D	74	GLY	3.3
1	E	58	ARG	3.2
3	J	8	DT	3.2
2	G	20	DA	3.1
1	E	60	LEU	3.1
1	D	9	VAL	3.1
1	B	72	ASP	3.1
2	I	18	DA	2.9
1	F	56	LEU	2.8
3	H	1	DT	2.7
1	F	43	LEU	2.7
1	E	125	HIS	2.6
3	J	19	DC	2.6
1	E	40	LEU	2.6
1	D	5	LYS	2.6
1	F	21	ARG	2.6
1	B	41	ALA	2.5
1	F	22	GLN	2.5
1	E	19	ALA	2.4
1	E	33	GLN	2.4
1	F	65	ALA	2.4
1	C	125	HIS	2.3
1	E	47	GLU	2.3
1	E	62	GLU	2.3
1	E	53	GLN	2.3
1	E	63	LEU	2.3
1	D	146	ASP	2.3
1	B	122	GLY	2.2
1	E	16	ALA	2.2
1	E	86	PRO	2.2
1	F	60	LEU	2.2
1	D	170	ARG	2.2
1	B	32	ALA	2.2
1	C	83	ASP	2.1
2	I	20	DA	2.1
1	A	51	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	78	TYR	2.1
1	F	49	ILE	2.1
1	B	146	ASP	2.0
1	B	35	ARG	2.0
2	I	1	DT	2.0
1	C	78	TYR	2.0
1	E	21	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

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	ARG	B	301	4/12	0.79	0.75	6.36	59,98,105,124	0
4	ARG	C	300	4/12	0.82	0.58	5.49	61,64,85,104	0
6	GOL	D	500	6/6	0.82	0.42	5.17	109,117,123,147	0
5	ACT	A	400	4/4	0.95	0.70	4.59	91,99,103,112	0
4	ARG	A	302	4/12	0.84	0.56	4.38	59,67,79,112	0
4	ARG	F	200	12/12	0.88	0.54	2.83	58,80,109,113	0
4	ARG	D	200	12/12	0.95	0.47	2.02	52,76,95,109	0
5	ACT	B	401	4/4	0.89	0.34	1.83	73,74,96,123	0
4	ARG	C	200	12/12	0.95	0.40	1.81	63,83,105,109	0
4	ARG	B	200	12/12	0.97	0.33	0.67	37,67,77,83	0
4	ARG	E	200	12/12	0.98	0.29	0.28	56,69,79,91	0
4	ARG	A	200	12/12	0.95	0.27	0.27	65,79,90,105	0

## 6.5 Other polymers

There are no such residues in this entry.