



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2024 – 09:47 AM EDT

PDB ID : 2AEG  
Title : X-Ray Crystal Structure of Protein Atu5096 from *Agrobacterium tumefaciens*.  
Northeast Structural Genomics Consortium Target AtR63.  
Authors : Forouhar, F.; Abashidze, M.; Kuzin, A.P.; Vorobiev, S.M.; Shastry, R.;  
Cooper, B.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast  
Structural Genomics Consortium (NESG)  
Deposited on : 2005-07-22  
Resolution : 2.30 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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

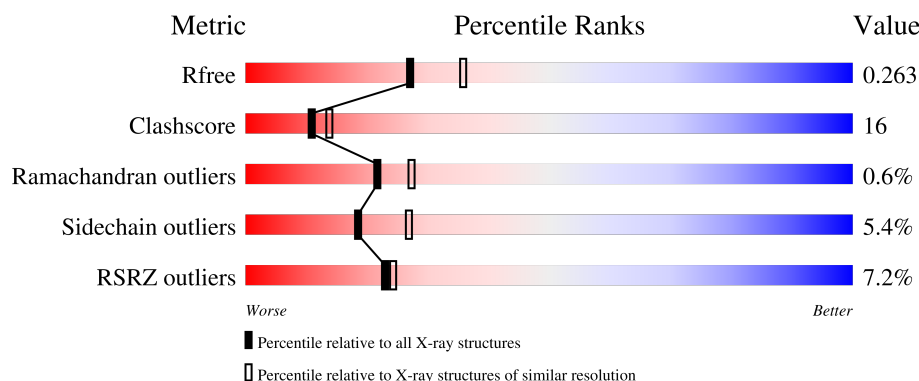
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	268	<div> <div>5%</div> <div> <div></div> <div>62%</div> <div>25%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	268	<div> <div>9%</div> <div> <div></div> <div>63%</div> <div>24%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	268	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>22%</div> <div>•</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6216 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 hypothetical protein AGR\_pAT\_140.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	Se	0	0	0
			1955	1248	348	349	2	8			
1	B	243	Total	C	N	O	S	Se	0	0	0
			1955	1248	348	349	2	8			
1	C	243	Total	C	N	O	S	Se	0	0	0
			1955	1248	348	349	2	8			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q8UKK6
A	7	MSE	MET	modified residue	UNP Q8UKK6
A	27	MSE	MET	modified residue	UNP Q8UKK6
A	32	MSE	MET	modified residue	UNP Q8UKK6
A	37	MSE	MET	modified residue	UNP Q8UKK6
A	91	MSE	MET	modified residue	UNP Q8UKK6
A	153	MSE	MET	modified residue	UNP Q8UKK6
A	198	MSE	MET	modified residue	UNP Q8UKK6
A	212	MSE	MET	modified residue	UNP Q8UKK6
A	258	ALA	-	cloning artifact	UNP Q8UKK6
A	259	ALA	-	cloning artifact	UNP Q8UKK6
A	260	ALA	-	cloning artifact	UNP Q8UKK6
A	261	LEU	-	cloning artifact	UNP Q8UKK6
A	262	GLU	-	cloning artifact	UNP Q8UKK6
A	263	HIS	-	expression tag	UNP Q8UKK6
A	264	HIS	-	expression tag	UNP Q8UKK6
A	265	HIS	-	expression tag	UNP Q8UKK6
A	266	HIS	-	expression tag	UNP Q8UKK6
A	267	HIS	-	expression tag	UNP Q8UKK6
A	268	HIS	-	expression tag	UNP Q8UKK6
B	1	MSE	MET	modified residue	UNP Q8UKK6
B	7	MSE	MET	modified residue	UNP Q8UKK6
B	27	MSE	MET	modified residue	UNP Q8UKK6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	32	MSE	MET	modified residue	UNP Q8UKK6
B	37	MSE	MET	modified residue	UNP Q8UKK6
B	91	MSE	MET	modified residue	UNP Q8UKK6
B	153	MSE	MET	modified residue	UNP Q8UKK6
B	198	MSE	MET	modified residue	UNP Q8UKK6
B	212	MSE	MET	modified residue	UNP Q8UKK6
B	258	ALA	-	cloning artifact	UNP Q8UKK6
B	259	ALA	-	cloning artifact	UNP Q8UKK6
B	260	ALA	-	cloning artifact	UNP Q8UKK6
B	261	LEU	-	cloning artifact	UNP Q8UKK6
B	262	GLU	-	cloning artifact	UNP Q8UKK6
B	263	HIS	-	expression tag	UNP Q8UKK6
B	264	HIS	-	expression tag	UNP Q8UKK6
B	265	HIS	-	expression tag	UNP Q8UKK6
B	266	HIS	-	expression tag	UNP Q8UKK6
B	267	HIS	-	expression tag	UNP Q8UKK6
B	268	HIS	-	expression tag	UNP Q8UKK6
C	1	MSE	MET	modified residue	UNP Q8UKK6
C	7	MSE	MET	modified residue	UNP Q8UKK6
C	27	MSE	MET	modified residue	UNP Q8UKK6
C	32	MSE	MET	modified residue	UNP Q8UKK6
C	37	MSE	MET	modified residue	UNP Q8UKK6
C	91	MSE	MET	modified residue	UNP Q8UKK6
C	153	MSE	MET	modified residue	UNP Q8UKK6
C	198	MSE	MET	modified residue	UNP Q8UKK6
C	212	MSE	MET	modified residue	UNP Q8UKK6
C	258	ALA	-	cloning artifact	UNP Q8UKK6
C	259	ALA	-	cloning artifact	UNP Q8UKK6
C	260	ALA	-	cloning artifact	UNP Q8UKK6
C	261	LEU	-	cloning artifact	UNP Q8UKK6
C	262	GLU	-	cloning artifact	UNP Q8UKK6
C	263	HIS	-	expression tag	UNP Q8UKK6
C	264	HIS	-	expression tag	UNP Q8UKK6
C	265	HIS	-	expression tag	UNP Q8UKK6
C	266	HIS	-	expression tag	UNP Q8UKK6
C	267	HIS	-	expression tag	UNP Q8UKK6
C	268	HIS	-	expression tag	UNP Q8UKK6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	122	Total O 122 122	0	0

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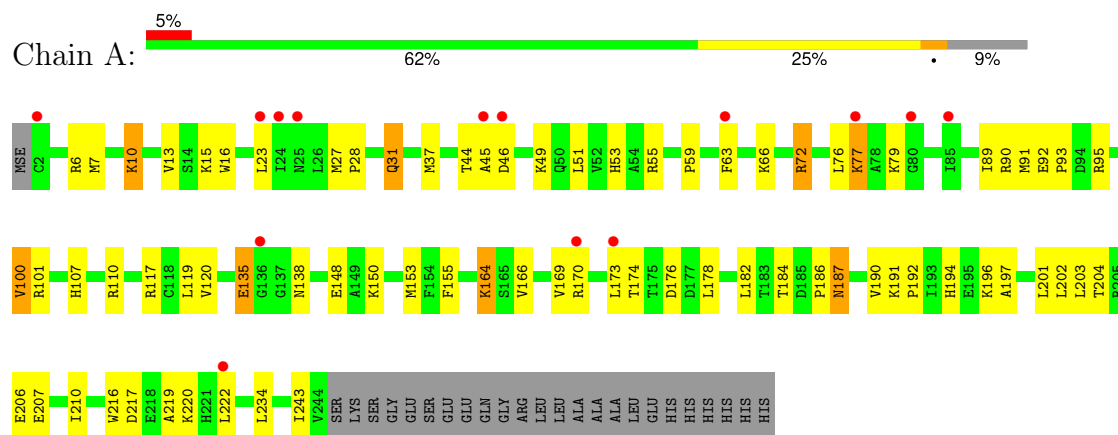
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	81	Total 81	O 81	0	0
2	C	148	Total 148	O 148	0	0

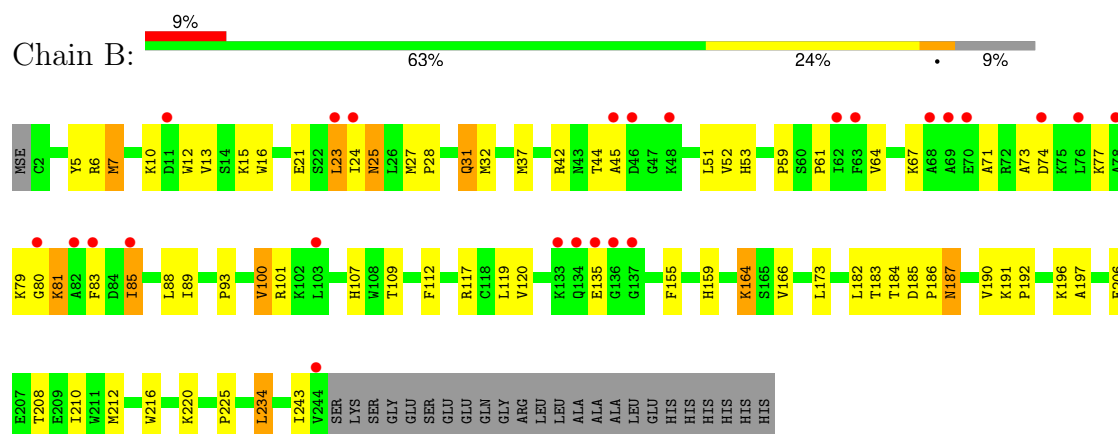
### 3 Residue-property plots

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.

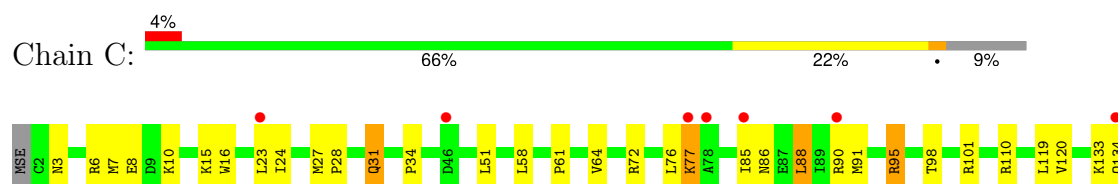
- Molecule 1: hypothetical protein AGR\_pAT\_140

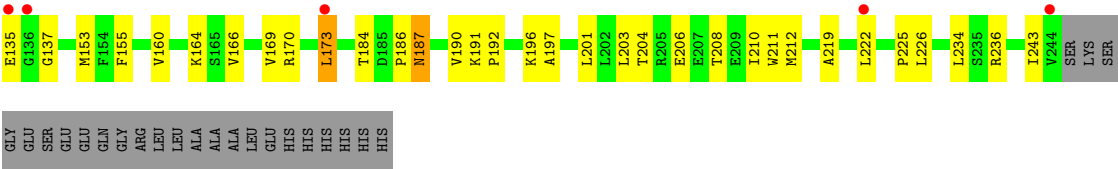


- Molecule 1: hypothetical protein AGR\_pAT\_140



- Molecule 1: hypothetical protein AGR\_pAT\_140





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	195.93Å 73.99Å 65.57Å 90.00° 106.21° 90.00°	Depositor
Resolution (Å)	29.81 – 2.30 29.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.1 (29.81-2.30) 97.3 (29.81-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.217 , 0.254 0.227 , 0.263	Depositor DCC
$R_{free}$ test set	3947 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6216	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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

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	0.36	0/2001	0.59	0/2705
1	B	0.37	0/2001	0.59	0/2705
1	C	0.38	0/2001	0.64	0/2705
All	All	0.37	0/6003	0.61	0/8115

There are no bond length outliers.

There are no bond angle outliers.

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	1955	0	1949	69	0
1	B	1955	0	1949	62	0
1	C	1955	0	1949	65	0
2	A	122	0	0	5	0
2	B	81	0	0	3	0
2	C	148	0	0	5	0
All	All	6216	0	5847	191	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 16.

All (191) 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:A:153:MSE:HE3	1:A:203:LEU:HD21	1.33	1.07
1:C:27:MSE:HG3	1:C:28:PRO:HD2	1.41	0.98
1:C:153:MSE:HE3	1:C:203:LEU:HD21	1.49	0.94
1:B:164:LYS:H	1:B:164:LYS:HE2	1.41	0.86
1:C:6:ARG:HE	1:C:31:GLN:NE2	1.74	0.84
1:B:186:PRO:HD3	1:B:197:ALA:HA	1.58	0.83
1:C:90:ARG:HB3	1:C:91:MSE:HE2	1.64	0.79
1:A:27:MSE:HG3	1:A:28:PRO:HD2	1.63	0.79
1:B:25:ASN:ND2	1:C:236:ARG:H	1.79	0.79
1:C:186:PRO:HD3	1:C:197:ALA:HA	1.66	0.78
1:C:153:MSE:HE2	1:C:201:LEU:HB3	1.68	0.76
1:C:164:LYS:HG2	1:C:173:LEU:CD1	2.16	0.75
1:A:153:MSE:HE1	1:A:201:LEU:HD13	1.67	0.75
1:C:120:VAL:HB	1:C:155:PHE:HB2	1.69	0.74
1:C:164:LYS:HG2	1:C:173:LEU:HD11	1.69	0.74
1:C:77:LYS:HA	1:C:77:LYS:NZ	2.04	0.73
1:A:72:ARG:HH11	1:A:72:ARG:HB2	1.52	0.72
1:A:164:LYS:HE2	1:A:164:LYS:H	1.52	0.72
1:B:101:ARG:HD3	1:B:183:THR:HG23	1.70	0.72
1:C:153:MSE:HE3	1:C:203:LEU:CD2	2.19	0.71
1:A:6:ARG:HE	1:A:31:GLN:NE2	1.89	0.71
1:C:24:ILE:HD11	1:C:51:LEU:HD22	1.74	0.70
1:A:153:MSE:HE2	1:A:201:LEU:HD22	1.73	0.70
1:B:6:ARG:HE	1:B:31:GLN:NE2	1.90	0.69
1:A:101:ARG:HH12	1:A:197:ALA:HB2	1.57	0.68
1:A:186:PRO:HD3	1:A:197:ALA:HA	1.76	0.68
1:C:77:LYS:HA	1:C:77:LYS:HZ1	1.57	0.68
1:A:10:LYS:HE3	1:A:10:LYS:H	1.59	0.67
1:B:77:LYS:HB2	1:B:83:PHE:HE1	1.60	0.66
1:A:37:MSE:HE3	1:A:53:HIS:HB3	1.77	0.66
1:A:101:ARG:NH1	1:A:197:ALA:HB2	2.09	0.66
1:A:153:MSE:HE3	1:A:203:LEU:CD2	2.20	0.66
1:B:120:VAL:HB	1:B:155:PHE:HB2	1.77	0.66
1:C:8:GLU:O	1:C:10:LYS:HD3	1.96	0.65
1:A:10:LYS:H	1:A:10:LYS:CE	2.09	0.65
1:B:164:LYS:H	1:B:164:LYS:CE	2.10	0.65
1:B:6:ARG:HE	1:B:31:GLN:HE22	1.44	0.65
1:B:100:VAL:HG13	1:B:182:LEU:HA	1.79	0.64
1:C:166:VAL:HG23	1:C:173:LEU:HD22	1.79	0.64
1:A:120:VAL:HB	1:A:155:PHE:HB2	1.79	0.64
1:B:61:PRO:HB2	1:B:64:VAL:HG23	1.80	0.64
1:A:206:GLU:O	1:A:210:ILE:HG12	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ILE:HD11	1:B:51:LEU:HD22	1.79	0.63
1:B:31:GLN:HE21	1:B:243:ILE:HG12	1.64	0.62
1:A:187:ASN:C	1:A:187:ASN:HD22	2.01	0.62
1:A:100:VAL:HG13	1:A:182:LEU:HA	1.82	0.62
1:C:211:TRP:CE3	1:C:222:LEU:HD11	2.34	0.62
1:C:196:LYS:O	1:C:197:ALA:HB2	2.00	0.61
1:A:153:MSE:HE2	1:A:201:LEU:HB3	1.83	0.61
1:C:101:ARG:NH1	1:C:197:ALA:HB2	2.17	0.60
1:B:10:LYS:HE2	1:C:243:ILE:O	2.02	0.60
1:C:187:ASN:HD22	1:C:187:ASN:C	2.05	0.59
1:A:72:ARG:O	1:A:76:LEU:HD13	2.01	0.59
1:B:184:THR:O	1:B:197:ALA:HB1	2.02	0.59
1:C:153:MSE:HE1	1:C:201:LEU:HD13	1.85	0.59
1:C:211:TRP:HE3	1:C:222:LEU:HD11	1.69	0.58
1:B:31:GLN:NE2	1:B:243:ILE:HG12	2.19	0.57
1:B:191:LYS:HB3	1:B:192:PRO:HD3	1.86	0.56
1:A:153:MSE:CE	1:A:201:LEU:HD13	2.35	0.56
1:B:37:MSE:HE3	1:B:53:HIS:HB3	1.86	0.56
1:B:117:ARG:HH11	1:B:117:ARG:HG3	1.69	0.56
1:B:6:ARG:CZ	1:B:243:ILE:HG23	2.35	0.56
1:A:90:ARG:CZ	1:A:91:MSE:HE3	2.36	0.56
1:A:79:LYS:HE2	2:A:374:HOH:O	2.06	0.56
1:B:119:LEU:HD13	1:B:212:MSE:SE	2.56	0.56
1:A:95:ARG:HG2	1:A:95:ARG:HH11	1.71	0.55
1:A:164:LYS:H	1:A:164:LYS:CE	2.19	0.55
1:A:6:ARG:HE	1:A:31:GLN:HE22	1.55	0.55
1:A:219:ALA:O	1:A:222:LEU:HG	2.05	0.55
1:B:42:ARG:HB2	1:B:159:HIS:CD2	2.41	0.55
1:B:71:ALA:HA	1:B:74:ASP:OD2	2.06	0.55
1:C:206:GLU:H	1:C:206:GLU:CD	2.09	0.55
1:A:202:LEU:HD21	1:A:222:LEU:HD13	1.88	0.55
1:A:44:THR:HG22	1:A:46:ASP:H	1.72	0.54
1:A:72:ARG:HB2	1:A:72:ARG:NH1	2.22	0.54
1:C:191:LYS:HB3	1:C:192:PRO:HD3	1.89	0.54
1:B:7:MSE:HE1	1:B:12:TRP:CD1	2.43	0.54
1:C:133:LYS:HE3	1:C:137:GLY:O	2.08	0.54
1:C:164:LYS:HG2	1:C:173:LEU:HD12	1.88	0.53
1:A:117:ARG:HG3	1:A:117:ARG:HH11	1.72	0.53
1:B:234:LEU:HD13	2:B:284:HOH:O	2.08	0.53
1:B:13:VAL:HG22	1:B:51:LEU:HD11	1.91	0.53
1:B:93:PRO:HA	1:B:166:VAL:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:MSE:SE	1:C:173:LEU:HD23	2.59	0.53
1:B:187:ASN:C	1:B:187:ASN:HD22	2.11	0.53
1:C:85:ILE:HG13	1:C:86:ASN:N	2.23	0.53
1:B:27:MSE:HG3	1:B:28:PRO:HD2	1.90	0.52
1:C:34:PRO:HB2	1:C:95:ARG:HH22	1.75	0.52
1:C:85:ILE:HG13	1:C:86:ASN:H	1.75	0.52
1:C:101:ARG:HH12	1:C:197:ALA:HB2	1.75	0.52
1:C:24:ILE:HD11	1:C:51:LEU:CD2	2.40	0.51
1:B:25:ASN:HD21	1:C:236:ARG:H	1.54	0.51
1:C:153:MSE:HG2	1:C:203:LEU:HD23	1.93	0.51
1:C:119:LEU:HD21	1:C:208:THR:HB	1.91	0.51
1:A:49:LYS:HE2	2:A:350:HOH:O	2.11	0.51
1:B:185:ASP:O	1:B:225:PRO:HB3	2.11	0.51
1:C:15:LYS:HG3	1:C:16:TRP:CD1	2.46	0.51
1:C:110:ARG:HD2	2:C:270:HOH:O	2.11	0.50
1:A:92:GLU:OE2	1:A:93:PRO:HD2	2.10	0.50
1:B:119:LEU:HD21	1:B:208:THR:HB	1.93	0.50
1:A:222:LEU:C	1:A:222:LEU:HD12	2.32	0.50
1:B:25:ASN:HD21	1:C:236:ARG:N	2.09	0.50
1:A:15:LYS:HG3	1:A:16:TRP:CD1	2.47	0.49
1:A:191:LYS:HB3	1:A:192:PRO:HD3	1.94	0.49
1:A:77:LYS:NZ	1:A:77:LYS:HA	2.27	0.48
1:B:196:LYS:O	1:B:197:ALA:HB2	2.14	0.48
1:C:6:ARG:HE	1:C:31:GLN:HE21	1.55	0.48
1:C:219:ALA:O	1:C:222:LEU:HG	2.13	0.48
1:A:187:ASN:ND2	1:A:190:VAL:H	2.10	0.48
1:B:101:ARG:HH12	1:B:197:ALA:HB2	1.78	0.48
1:B:10:LYS:HD2	1:B:10:LYS:H	1.77	0.48
1:B:42:ARG:HB2	1:B:159:HIS:NE2	2.28	0.48
1:B:59:PRO:O	1:B:107:HIS:HE1	1.97	0.48
1:C:201:LEU:HB2	1:C:226:LEU:HD11	1.95	0.48
1:A:66:LYS:HG3	1:A:89:ILE:HD11	1.96	0.48
1:B:101:ARG:NH1	1:B:197:ALA:HB2	2.29	0.48
1:B:187:ASN:ND2	1:B:190:VAL:H	2.12	0.47
1:A:196:LYS:O	1:A:197:ALA:HB2	2.15	0.47
1:C:184:THR:O	1:C:197:ALA:HB1	2.14	0.47
1:A:164:LYS:HA	1:A:174:THR:O	2.13	0.47
1:B:184:THR:OG1	1:B:185:ASP:N	2.48	0.47
1:A:13:VAL:HG22	1:A:51:LEU:HD11	1.97	0.47
1:B:25:ASN:ND2	1:C:236:ARG:N	2.56	0.47
1:B:67:LYS:HE3	2:B:312:HOH:O	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ILE:HG21	1:B:52:VAL:HA	1.95	0.46
1:B:164:LYS:H	1:B:164:LYS:CD	2.28	0.46
1:B:109:THR:HA	1:B:112:PHE:CD2	2.50	0.46
1:C:204:THR:OG1	1:C:206:GLU:HG2	2.16	0.46
1:C:206:GLU:O	1:C:210:ILE:HG12	2.16	0.46
1:A:59:PRO:O	1:A:107:HIS:HE1	1.99	0.45
1:A:72:ARG:HH11	1:A:72:ARG:CB	2.24	0.45
1:C:58:LEU:HD22	1:C:160:VAL:HG23	1.98	0.45
1:B:73:ALA:HB2	1:B:88:LEU:CD2	2.47	0.45
1:B:206:GLU:O	1:B:210:ILE:HG12	2.16	0.45
1:C:187:ASN:C	1:C:187:ASN:ND2	2.70	0.45
1:A:110:ARG:HD2	2:A:271:HOH:O	2.15	0.45
1:B:5:TYR:CZ	1:B:32:MSE:HG3	2.51	0.45
1:B:42:ARG:HD2	1:B:159:HIS:CE1	2.52	0.45
1:A:100:VAL:CG1	1:A:182:LEU:HD12	2.47	0.45
1:A:93:PRO:HA	1:A:166:VAL:O	2.17	0.44
1:A:95:ARG:HG2	1:A:95:ARG:NH1	2.32	0.44
1:C:225:PRO:HG2	2:C:342:HOH:O	2.17	0.44
1:A:117:ARG:HG3	1:A:117:ARG:NH1	2.32	0.44
1:C:72:ARG:O	1:C:76:LEU:HD13	2.17	0.44
1:C:153:MSE:HE2	1:C:201:LEU:HD22	1.98	0.44
1:C:170:ARG:NH1	1:C:170:ARG:HB3	2.32	0.44
1:A:170:ARG:HB3	1:A:170:ARG:NH1	2.32	0.44
1:C:61:PRO:HB2	1:C:64:VAL:HG23	1.99	0.44
1:B:44:THR:HG22	1:B:45:ALA:N	2.33	0.44
1:C:77:LYS:HE3	2:C:328:HOH:O	2.18	0.44
1:A:31:GLN:HE21	1:A:31:GLN:HB2	1.61	0.44
1:A:204:THR:OG1	1:A:207:GLU:HG3	2.17	0.44
1:C:27:MSE:CG	1:C:28:PRO:HD2	2.31	0.44
1:A:101:ARG:NH1	1:A:197:ALA:CB	2.81	0.43
1:B:10:LYS:HD2	1:B:10:LYS:N	2.34	0.43
1:A:63:PHE:HB2	2:A:357:HOH:O	2.18	0.43
1:A:194:HIS:CE1	1:A:196:LYS:HB3	2.53	0.43
1:B:85:ILE:HD11	1:B:89:ILE:HD11	2.01	0.43
1:C:6:ARG:HH21	1:C:31:GLN:HE22	1.65	0.43
1:C:196:LYS:O	1:C:197:ALA:CB	2.66	0.43
1:B:117:ARG:HG3	1:B:117:ARG:NH1	2.31	0.43
1:C:90:ARG:HG3	2:C:369:HOH:O	2.17	0.43
1:A:55:ARG:HB3	1:A:178:LEU:HD23	2.00	0.43
1:B:21:GLU:O	1:B:23:LEU:HD23	2.19	0.43
1:C:88:LEU:HD13	2:C:388:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:HD13	1:C:212:MSE:SE	2.69	0.43
1:A:217:ASP:HB2	2:A:274:HOH:O	2.18	0.42
1:A:164:LYS:H	1:A:164:LYS:CD	2.32	0.42
1:C:153:MSE:CE	1:C:201:LEU:HB3	2.45	0.42
1:C:187:ASN:ND2	1:C:190:VAL:H	2.17	0.42
1:A:31:GLN:HE21	1:A:243:ILE:HG12	1.84	0.42
1:B:183:THR:HG21	2:B:272:HOH:O	2.19	0.42
1:B:80:GLY:O	1:B:81:LYS:HG2	2.19	0.42
1:A:169:VAL:HG13	1:A:170:ARG:N	2.35	0.42
1:C:3:ASN:ND2	1:C:98:THR:OG1	2.53	0.42
1:A:150:LYS:HG3	1:A:234:LEU:HD11	2.02	0.41
1:B:216:TRP:O	1:B:220:LYS:HG2	2.21	0.41
1:A:148:GLU:HA	1:A:234:LEU:HD21	2.03	0.41
1:B:15:LYS:HG3	1:B:16:TRP:CD1	2.56	0.41
1:A:44:THR:HG22	1:A:45:ALA:N	2.36	0.41
1:A:138:ASN:HD22	1:A:138:ASN:HA	1.64	0.41
1:B:10:LYS:H	1:B:10:LYS:CD	2.33	0.41
1:B:23:LEU:O	1:B:24:ILE:HG23	2.21	0.41
1:C:169:VAL:HG13	1:C:170:ARG:N	2.35	0.41
1:A:66:LYS:HG3	1:A:89:ILE:CD1	2.51	0.40
1:A:187:ASN:C	1:A:187:ASN:ND2	2.70	0.40
1:B:73:ALA:HB1	1:B:83:PHE:CZ	2.56	0.40
1:C:204:THR:HB	1:C:206:GLU:OE2	2.21	0.40
1:A:216:TRP:CE2	1:A:220:LYS:HB3	2.56	0.40
1:A:100:VAL:HG11	1:A:182:LEU:HD12	2.03	0.40
1:A:184:THR:O	1:A:197:ALA:HB1	2.21	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	241/268 (90%)	229 (95%)	11 (5%)	1 (0%)	30	39
1	B	241/268 (90%)	219 (91%)	20 (8%)	2 (1%)	16	20
1	C	241/268 (90%)	230 (95%)	10 (4%)	1 (0%)	30	39
All	All	723/804 (90%)	678 (94%)	41 (6%)	4 (1%)	22	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	79	LYS
1	B	135	GLU
1	C	135	GLU
1	A	135	GLU

### 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	209/220 (95%)	196 (94%)	13 (6%)	15	22
1	B	209/220 (95%)	198 (95%)	11 (5%)	19	28
1	C	209/220 (95%)	199 (95%)	10 (5%)	21	32
All	All	627/660 (95%)	593 (95%)	34 (5%)	18	27

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	MSE
1	A	10	LYS
1	A	23	LEU
1	A	31	GLN
1	A	72	ARG
1	A	77	LYS
1	A	100	VAL
1	A	119	LEU
1	A	135	GLU

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Mol	Chain	Res	Type
1	A	164	LYS
1	A	173	LEU
1	A	176	ASP
1	A	187	ASN
1	B	7	MSE
1	B	23	LEU
1	B	25	ASN
1	B	31	GLN
1	B	81	LYS
1	B	85	ILE
1	B	100	VAL
1	B	164	LYS
1	B	173	LEU
1	B	187	ASN
1	B	234	LEU
1	C	7	MSE
1	C	23	LEU
1	C	31	GLN
1	C	77	LYS
1	C	88	LEU
1	C	95	ARG
1	C	134	GLN
1	C	173	LEU
1	C	187	ASN
1	C	234	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	31	GLN
1	A	107	HIS
1	A	138	ASN
1	A	187	ASN
1	A	194	HIS
1	A	221	HIS
1	B	3	ASN
1	B	25	ASN
1	B	31	GLN
1	B	107	HIS
1	B	116	HIS
1	B	138	ASN

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Mol	Chain	Res	Type
1	B	162	GLN
1	B	187	ASN
1	B	194	HIS
1	C	3	ASN
1	C	31	GLN
1	C	99	ASN
1	C	107	HIS
1	C	138	ASN
1	C	187	ASN
1	C	194	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](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 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	235/268 (87%)	0.32	14 (5%) 29 31	14, 28, 53, 57	0
1	B	235/268 (87%)	0.64	25 (10%) 13 14	11, 33, 54, 64	0
1	C	235/268 (87%)	0.13	12 (5%) 34 35	10, 24, 46, 61	0
All	All	705/804 (87%)	0.36	51 (7%) 23 24	10, 28, 52, 64	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	80	GLY	4.7
1	B	136	GLY	3.6
1	C	23	LEU	3.5
1	A	136	GLY	3.3
1	B	76	LEU	3.3
1	C	134	GLN	3.1
1	B	11	ASP	3.0
1	B	45	ALA	3.0
1	C	222	LEU	3.0
1	B	23	LEU	2.9
1	A	46	ASP	2.9
1	C	78	ALA	2.9
1	A	85	ILE	2.9
1	B	82	ALA	2.8
1	A	173	LEU	2.8
1	C	85	ILE	2.7
1	B	134	GLN	2.7
1	B	137	GLY	2.7
1	B	46	ASP	2.7
1	A	23	LEU	2.6
1	A	45	ALA	2.5
1	C	244	VAL	2.5
1	A	2	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	133	LYS	2.4
1	B	63	PHE	2.4
1	B	244	VAL	2.4
1	A	63	PHE	2.4
1	B	62	ILE	2.4
1	A	222	LEU	2.4
1	A	77	LYS	2.4
1	B	74	ASP	2.4
1	B	69	ALA	2.4
1	C	77	LYS	2.3
1	B	135	GLU	2.3
1	C	135	GLU	2.3
1	B	85	ILE	2.3
1	A	24	ILE	2.3
1	B	24	ILE	2.2
1	A	170	ARG	2.2
1	B	83	PHE	2.2
1	B	48	LYS	2.2
1	A	25	ASN	2.2
1	C	136	GLY	2.1
1	A	80	GLY	2.1
1	C	90	ARG	2.1
1	B	103	LEU	2.1
1	C	46	ASP	2.1
1	C	173	LEU	2.1
1	B	68	ALA	2.1
1	B	70	GLU	2.0
1	B	78	ALA	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.