



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:21 pm GMT

PDB ID : 3OBY  
Title : Crystal structure of Archaeoglobus fulgidus Pelota reveals inter-domain structural plasticity  
Authors : Lee, H.H.; Jang, J.Y.; Yoon, H.-J.; Kim, S.J.; Suh, S.W.  
Deposited on : 2010-08-09  
Resolution : 2.90 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

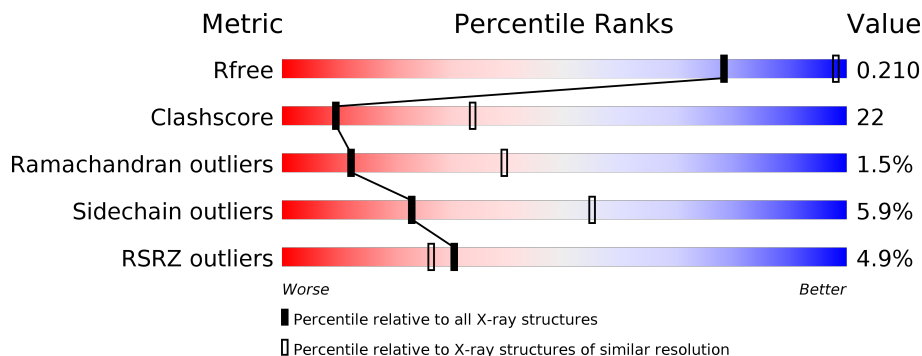
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	352	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>26%</div> <div>• 10%</div> </div> </div>
1	B	352	<div> <div>6%</div> <div> <div></div> <div>51%</div> <div>34%</div> <div>• • 10%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5312 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 Protein pelota homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2553	1633	441	473	6			
1	B	316	Total	C	N	O	S	0	0	0
			2547	1631	437	473	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	345	LEU	-	EXPRESSION TAG	UNP O29421
A	346	GLU	-	EXPRESSION TAG	UNP O29421
A	347	HIS	-	EXPRESSION TAG	UNP O29421
A	348	HIS	-	EXPRESSION TAG	UNP O29421
A	349	HIS	-	EXPRESSION TAG	UNP O29421
A	350	HIS	-	EXPRESSION TAG	UNP O29421
A	351	HIS	-	EXPRESSION TAG	UNP O29421
A	352	HIS	-	EXPRESSION TAG	UNP O29421
B	345	LEU	-	EXPRESSION TAG	UNP O29421
B	346	GLU	-	EXPRESSION TAG	UNP O29421
B	347	HIS	-	EXPRESSION TAG	UNP O29421
B	348	HIS	-	EXPRESSION TAG	UNP O29421
B	349	HIS	-	EXPRESSION TAG	UNP O29421
B	350	HIS	-	EXPRESSION TAG	UNP O29421
B	351	HIS	-	EXPRESSION TAG	UNP O29421
B	352	HIS	-	EXPRESSION TAG	UNP O29421

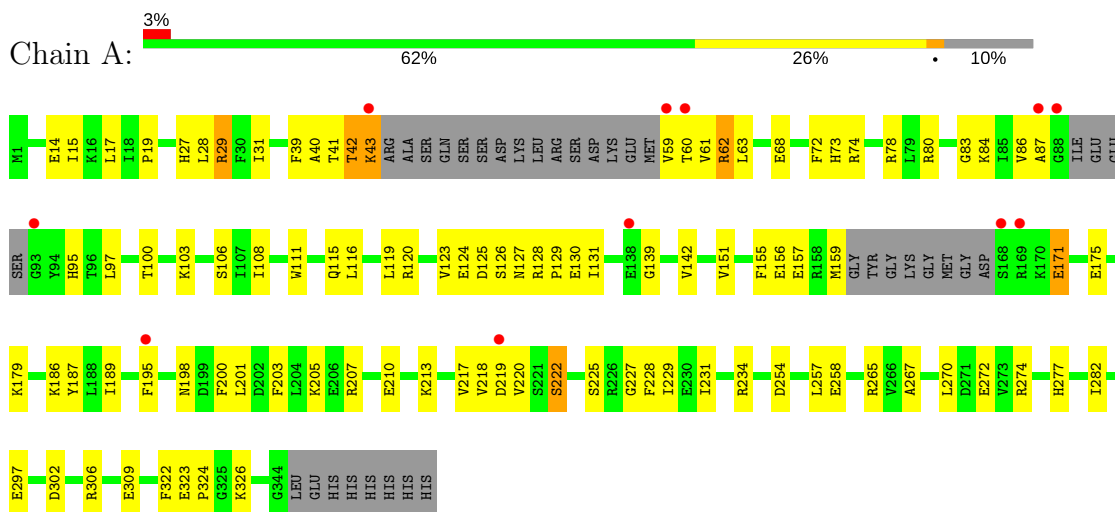
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	146	Total	O	0	0
			146	146		
2	B	66	Total	O	0	0
			66	66		

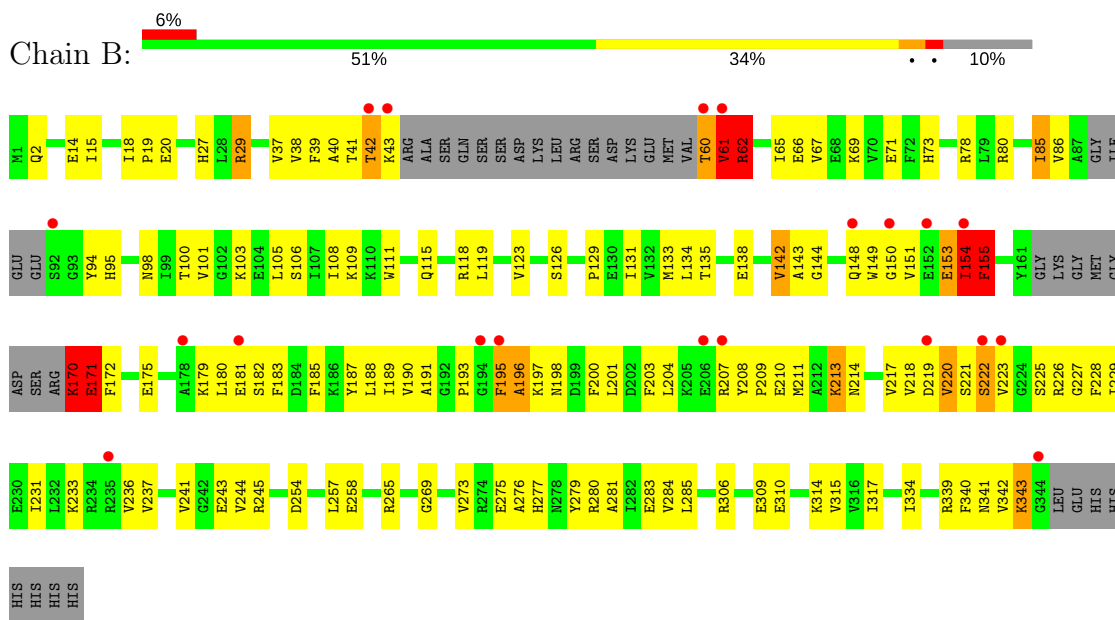
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Protein pelota homolog



#### • Molecule 1: Protein pelota homolog



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.24Å 66.69Å 98.38Å 90.00° 107.29° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 14.98 – 2.89	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.90) 95.6 (14.98-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	39.36 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.209 , 0.279 0.218 , 0.210	Depositor DCC
$R_{free}$ test set	1771 reflections (9.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 71.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	5312	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.59% 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	0.39	0/2590	0.63	1/3477 (0.0%)
1	B	0.47	4/2585 (0.2%)	0.83	12/3471 (0.3%)
All	All	0.43	4/5175 (0.1%)	0.74	13/6948 (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
1	B	1	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	195	PHE	CA-CB	-5.66	1.41	1.53
1	B	196	ALA	CA-CB	-5.55	1.40	1.52
1	B	195	PHE	C-O	5.23	1.33	1.23
1	B	61	VAL	CB-CG1	5.13	1.63	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	LYS	CA-CB-CG	-12.34	86.25	113.40
1	B	170	LYS	CA-C-N	-12.33	90.07	117.20
1	B	61	VAL	N-CA-CB	-12.08	84.92	111.50
1	B	61	VAL	CA-CB-CG2	10.07	126.01	110.90
1	A	42	THR	C-N-CA	-8.07	101.52	121.70
1	B	170	LYS	CB-CA-C	7.06	124.52	110.40
1	B	171	GLU	N-CA-CB	6.95	123.11	110.60
1	B	153	GLU	C-N-CA	6.31	137.48	121.70
1	B	62	ARG	CA-C-N	-5.65	104.77	117.20
1	B	195	PHE	CA-C-N	5.43	129.16	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	VAL	CA-CB-CG1	5.38	118.97	110.90
1	B	149	TRP	N-CA-C	-5.13	97.16	111.00
1	B	62	ARG	N-CA-CB	5.12	119.81	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	154	ILE	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	154	ILE	Mainchain
1	B	170	LYS	Mainchain

## 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	2553	0	2599	88	0
1	B	2547	0	2586	135	0
2	A	146	0	0	6	0
2	B	66	0	0	5	0
All	All	5312	0	5185	223	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 22.

All (223) 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:B:175:GLU:O	1:B:179:LYS:HG3	1.20	1.34
1:B:60:THR:CB	1:B:61:VAL:HG12	1.70	1.22
1:B:60:THR:HB	1:B:61:VAL:CG1	1.73	1.18
1:B:42:THR:HB	1:B:61:VAL:HG11	1.26	1.14
1:B:143:ALA:O	1:B:153:GLU:O	1.65	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:GLU:O	1:B:179:LYS:CG	2.00	1.08
1:B:42:THR:HB	1:B:61:VAL:CG1	1.84	1.08
1:B:343:LYS:HA	1:B:343:LYS:HE3	1.39	1.00
1:B:144:GLY:HA2	1:B:153:GLU:O	1.64	0.98
1:A:157:GLU:OE1	1:A:179:LYS:NZ	1.97	0.97
1:B:342:VAL:HG23	1:B:343:LYS:H	1.29	0.97
1:A:14:GLU:HB2	1:A:108:ILE:HG12	1.46	0.95
1:B:60:THR:O	1:B:61:VAL:HB	1.54	0.92
1:B:60:THR:HB	1:B:61:VAL:HG12	0.94	0.92
1:B:42:THR:O	1:B:43:LYS:HG3	1.69	0.92
1:A:201:LEU:HG	1:A:205:LYS:HE3	1.49	0.91
1:B:41:THR:HA	1:B:62:ARG:HB2	1.52	0.90
1:B:171:GLU:OE1	1:B:171:GLU:HA	1.72	0.90
1:A:42:THR:HG21	1:A:95:HIS:NE2	1.88	0.87
1:B:170:LYS:HD3	1:B:171:GLU:H	1.40	0.84
1:A:171:GLU:OE1	1:A:171:GLU:HA	1.75	0.83
1:B:175:GLU:HB3	1:B:179:LYS:HE3	1.59	0.83
1:B:42:THR:CB	1:B:61:VAL:HG11	2.09	0.80
1:B:193:PRO:HB3	1:B:221:SER:HA	1.64	0.79
1:B:306:ARG:O	1:B:310:GLU:HG3	1.82	0.79
1:A:129:PRO:HG2	1:A:131:ILE:HD11	1.65	0.79
1:A:142:VAL:HG22	1:A:156:GLU:HG2	1.64	0.78
1:B:197:LYS:NZ	1:B:219:ASP:HA	2.00	0.77
1:A:43:LYS:HG3	1:A:60:THR:HG22	1.69	0.74
1:B:220:VAL:HG22	1:B:222:SER:H	1.52	0.74
1:A:222:SER:HB2	1:A:227:GLY:HA2	1.70	0.73
1:A:43:LYS:HG3	1:A:60:THR:CG2	2.19	0.73
1:B:277:HIS:O	1:B:280:ARG:HD2	1.88	0.73
1:B:73:HIS:CE1	1:B:80:ARG:HB2	2.24	0.72
1:A:129:PRO:HB2	1:A:186:LYS:HD2	1.71	0.72
1:B:78:ARG:HG2	1:B:100:THR:HG22	1.70	0.72
1:A:129:PRO:CB	1:A:186:LYS:HD2	2.19	0.72
1:A:195:PHE:HA	1:A:198:ASN:HD22	1.53	0.71
1:B:42:THR:O	1:B:43:LYS:CG	2.39	0.71
1:B:155:PHE:CD2	1:B:155:PHE:C	2.64	0.71
1:B:342:VAL:HG23	1:B:343:LYS:N	2.03	0.71
1:B:154:ILE:O	1:B:155:PHE:HB3	1.91	0.70
1:B:171:GLU:OE1	1:B:171:GLU:CA	2.40	0.70
1:B:175:GLU:O	1:B:179:LYS:CD	2.40	0.70
1:B:254:ASP:O	1:B:258:GLU:HG3	1.93	0.69
1:B:144:GLY:CA	1:B:153:GLU:O	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:PHE:HD2	1:B:155:PHE:C	1.97	0.68
1:B:201:LEU:HD22	1:B:217:VAL:HG23	1.75	0.68
1:B:170:LYS:HD3	1:B:171:GLU:N	2.03	0.67
1:B:133:MET:CE	1:B:231:ILE:HB	2.24	0.67
1:A:130:GLU:H	1:A:186:LYS:HZ2	1.42	0.66
1:B:197:LYS:HZ2	1:B:219:ASP:HA	1.59	0.66
1:B:42:THR:HB	1:B:61:VAL:HG13	1.75	0.66
1:A:139:GLY:HA3	1:A:159:MET:HB2	1.76	0.66
1:B:154:ILE:HD11	1:B:183:PHE:CD1	2.30	0.66
1:A:220:VAL:HG21	1:A:231:ILE:HD13	1.78	0.65
1:B:126:SER:HB2	2:B:401:HOH:O	1.94	0.65
1:A:43:LYS:HD2	1:A:43:LYS:N	2.11	0.65
1:A:139:GLY:CA	1:A:159:MET:HB2	2.27	0.65
1:A:129:PRO:HB2	1:A:186:LYS:HG3	1.80	0.64
1:B:134:LEU:HD12	1:B:143:ALA:HB2	1.78	0.64
1:B:42:THR:H	1:B:61:VAL:HG13	1.62	0.64
1:B:85:ILE:HD11	1:B:95:HIS:HB2	1.81	0.62
1:A:68:GLU:HG3	1:A:83:GLY:HA2	1.82	0.62
1:B:171:GLU:OE1	1:B:171:GLU:N	2.33	0.62
1:A:151:VAL:HG21	1:A:228:PHE:HB3	1.82	0.61
1:A:201:LEU:HD22	1:A:217:VAL:HG23	1.82	0.61
1:A:282:ILE:HG12	2:A:479:HOH:O	1.99	0.61
1:A:41:THR:HA	1:A:62:ARG:HA	1.83	0.59
1:B:317:ILE:HD12	1:B:317:ILE:N	2.17	0.59
1:B:143:ALA:C	1:B:153:GLU:O	2.39	0.59
1:B:275:GLU:O	1:B:279:TYR:HD2	1.85	0.59
1:A:218:VAL:HG12	1:A:220:VAL:H	1.67	0.59
1:B:133:MET:HE2	1:B:228:PHE:HA	1.85	0.58
1:B:343:LYS:CA	1:B:343:LYS:HE3	2.24	0.58
1:A:129:PRO:HB2	1:A:186:LYS:CD	2.33	0.58
1:B:133:MET:HE3	1:B:231:ILE:HB	1.84	0.58
1:A:254:ASP:O	1:A:258:GLU:HG3	2.04	0.58
1:B:219:ASP:O	1:B:220:VAL:HB	2.03	0.58
1:B:129:PRO:O	1:B:131:ILE:HG13	2.05	0.57
1:B:175:GLU:C	1:B:179:LYS:HG3	2.16	0.57
1:B:237:VAL:O	1:B:241:VAL:HG23	2.05	0.57
1:B:135:THR:OG1	1:B:142:VAL:HG13	2.04	0.56
1:B:119:LEU:O	1:B:123:VAL:HG23	2.05	0.56
1:B:154:ILE:HD11	1:B:183:PHE:HD1	1.70	0.56
1:B:27:HIS:HE1	1:B:309:GLU:OE2	1.89	0.56
1:A:219:ASP:HB3	1:A:234:ARG:HH12	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:PHE:O	1:B:203:PHE:HB3	2.05	0.55
1:A:302:ASP:O	1:A:306:ARG:HG3	2.06	0.55
1:B:134:LEU:CD1	1:B:143:ALA:HB2	2.37	0.55
1:B:175:GLU:O	1:B:179:LYS:HD2	2.06	0.55
1:B:189:ILE:N	1:B:189:ILE:HD12	2.22	0.55
1:A:129:PRO:HB2	1:A:186:LYS:CG	2.37	0.54
1:B:343:LYS:HA	1:B:343:LYS:CE	2.25	0.54
1:B:14:GLU:HB2	1:B:108:ILE:HG12	1.89	0.54
1:A:29:ARG:HD3	1:A:29:ARG:C	2.28	0.54
1:A:130:GLU:H	1:A:186:LYS:NZ	2.05	0.53
1:B:187:TYR:HE1	1:B:214:ASN:HD22	1.56	0.53
1:A:78:ARG:HG2	1:A:100:THR:HG22	1.90	0.53
1:B:148:GLN:C	1:B:150:GLY:H	2.07	0.53
1:A:227:GLY:O	1:A:231:ILE:HG12	2.09	0.53
1:B:42:THR:O	1:B:43:LYS:CB	2.57	0.53
1:A:189:ILE:HD12	1:A:189:ILE:N	2.24	0.53
1:A:195:PHE:HA	1:A:198:ASN:ND2	2.23	0.53
1:B:180:LEU:C	1:B:182:SER:H	2.11	0.52
1:B:225:SER:O	1:B:229:ILE:HG12	2.09	0.52
1:A:73:HIS:CE1	1:A:80:ARG:HB2	2.45	0.52
1:B:39:PHE:HB2	1:B:106:SER:HB2	1.91	0.52
1:B:38:VAL:HB	1:B:65:ILE:HD11	1.92	0.52
1:A:42:THR:O	1:A:60:THR:HG22	2.09	0.51
1:B:342:VAL:CG2	1:B:343:LYS:H	2.11	0.51
1:B:60:THR:C	1:B:61:VAL:CG1	2.73	0.51
1:B:20:GLU:OE1	1:B:126:SER:OG	2.28	0.51
1:B:78:ARG:HG2	1:B:100:THR:CG2	2.40	0.51
1:A:42:THR:CG2	1:A:95:HIS:NE2	2.67	0.51
1:A:267:ALA:HA	1:A:272:GLU:OE1	2.11	0.51
1:A:225:SER:O	1:A:229:ILE:HG12	2.12	0.50
1:B:65:ILE:O	1:B:65:ILE:HD12	2.11	0.50
1:A:282:ILE:HD12	1:A:282:ILE:N	2.26	0.50
1:B:133:MET:HE3	1:B:231:ILE:CB	2.42	0.50
1:A:86:VAL:HG13	1:A:87:ALA:N	2.26	0.49
1:B:2:GLN:HG3	1:B:20:GLU:OE2	2.11	0.49
1:B:210:GLU:O	1:B:213:LYS:HG3	2.12	0.49
1:B:245:ARG:HD3	2:B:403:HOH:O	2.13	0.49
1:A:40:ALA:O	1:A:62:ARG:HA	2.13	0.49
1:B:2:GLN:HB2	1:B:18:ILE:HB	1.95	0.49
1:A:120:ARG:HD2	2:A:357:HOH:O	2.13	0.49
1:B:281:ALA:O	1:B:339:ARG:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:VAL:HG13	1:A:63:LEU:HD13	1.94	0.49
1:A:201:LEU:CG	1:A:205:LYS:HE3	2.33	0.48
1:A:200:PHE:O	1:A:203:PHE:HB3	2.13	0.48
1:A:29:ARG:HD3	1:A:29:ARG:O	2.13	0.48
1:A:40:ALA:HB3	1:A:97:LEU:HD22	1.96	0.48
1:B:191:ALA:HB2	1:B:218:VAL:CG2	2.43	0.48
1:B:226:ARG:HG3	1:B:226:ARG:HH11	1.78	0.48
1:B:66:GLU:HB2	1:B:86:VAL:CG1	2.44	0.48
1:A:27:HIS:HE1	1:A:309:GLU:OE2	1.96	0.48
1:A:31:ILE:HD12	1:A:115:GLN:HB3	1.94	0.48
1:A:42:THR:O	1:A:60:THR:HA	2.14	0.48
1:B:276:ALA:HA	1:B:342:VAL:HG11	1.95	0.48
1:A:322:PHE:O	1:A:326:LYS:HG3	2.14	0.48
1:A:41:THR:HG22	1:A:62:ARG:HB2	1.95	0.48
1:B:222:SER:OG	1:B:227:GLY:HA2	2.13	0.48
1:A:19:PRO:HB3	1:A:28:LEU:HD11	1.96	0.47
1:A:277:HIS:HB2	2:A:479:HOH:O	2.13	0.47
1:A:43:LYS:HG3	1:A:60:THR:HG23	1.94	0.47
1:B:42:THR:HG23	1:B:43:LYS:N	2.28	0.47
1:B:133:MET:HE1	1:B:231:ILE:HB	1.96	0.47
1:A:270:LEU:HG	1:A:274:ARG:HD2	1.96	0.47
1:B:265:ARG:NH1	1:B:340:PHE:HA	2.29	0.47
1:B:85:ILE:HD11	1:B:95:HIS:CB	2.45	0.47
1:A:131:ILE:CD1	1:A:187:TYR:HB2	2.44	0.47
1:B:133:MET:CE	1:B:231:ILE:HD12	2.45	0.47
1:A:74:ARG:HD3	1:A:297:GLU:OE2	2.15	0.46
1:B:94:TYR:N	1:B:94:TYR:CD1	2.82	0.46
1:B:153:GLU:HG2	1:B:155:PHE:H	1.80	0.46
1:B:222:SER:OG	1:B:226:ARG:HG2	2.15	0.46
1:B:60:THR:C	1:B:61:VAL:HG12	2.32	0.46
1:B:225:SER:HA	1:B:228:PHE:CD2	2.49	0.46
1:B:283:GLU:HG2	1:B:284:VAL:HG23	1.97	0.46
1:A:129:PRO:HG2	1:A:131:ILE:CD1	2.41	0.46
1:A:15:ILE:HD12	1:A:111:TRP:CZ2	2.51	0.46
1:A:218:VAL:HG12	1:A:219:ASP:N	2.31	0.46
1:A:131:ILE:HD12	1:A:187:TYR:HB2	1.98	0.45
1:A:119:LEU:O	1:A:123:VAL:HG23	2.16	0.45
1:B:281:ALA:HB2	1:B:340:PHE:CE2	2.51	0.45
1:B:285:LEU:HD11	1:B:334:ILE:HD11	1.99	0.45
1:A:42:THR:HG21	1:A:95:HIS:CD2	2.49	0.45
1:B:109:LYS:NZ	1:B:115:GLN:HE22	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PHE:HB3	2:A:415:HOH:O	2.17	0.45
1:A:277:HIS:HA	1:A:282:ILE:HD13	1.98	0.44
1:B:209:PRO:O	1:B:213:LYS:HG2	2.17	0.44
1:B:181:GLU:HB2	1:B:211:MET:HE1	1.99	0.44
1:A:123:VAL:C	1:A:125:ASP:H	2.21	0.44
1:B:193:PRO:HD3	1:B:222:SER:O	2.17	0.44
1:B:231:ILE:HG23	1:B:236:VAL:HG21	1.99	0.44
1:A:265:ARG:HG3	1:A:265:ARG:HH21	1.83	0.44
1:B:101:VAL:O	1:B:101:VAL:HG23	2.18	0.44
1:B:133:MET:CE	1:B:228:PHE:HA	2.48	0.44
1:B:73:HIS:CE1	1:B:98:ASN:ND2	2.85	0.44
1:A:175:GLU:O	1:A:179:LYS:HG2	2.18	0.43
1:B:42:THR:CG2	1:B:61:VAL:HG11	2.47	0.43
1:A:39:PHE:HB2	1:A:106:SER:HB2	2.00	0.43
1:A:42:THR:O	1:A:43:LYS:CB	2.65	0.43
1:B:15:ILE:HD12	1:B:111:TRP:CZ2	2.53	0.43
1:A:323:GLU:HB2	1:A:324:PRO:HD3	2.01	0.43
1:A:84:LYS:HB3	1:A:84:LYS:NZ	2.34	0.43
1:B:180:LEU:C	1:B:182:SER:N	2.72	0.43
1:B:118:ARG:HD3	1:B:118:ARG:O	2.17	0.43
1:B:37:VAL:HA	1:B:65:ILE:O	2.19	0.43
1:A:155:PHE:CD2	1:A:179:LYS:HD2	2.54	0.42
1:A:86:VAL:CG1	1:A:87:ALA:N	2.81	0.42
1:B:315:VAL:HG12	1:B:317:ILE:CD1	2.49	0.42
1:B:197:LYS:HG3	1:B:198:ASN:N	2.34	0.42
1:B:40:ALA:C	1:B:62:ARG:HG3	2.40	0.42
1:B:109:LYS:HZ1	1:B:115:GLN:HE22	1.67	0.42
1:B:195:PHE:O	1:B:196:ALA:C	2.58	0.42
1:B:29:ARG:C	1:B:29:ARG:HD3	2.40	0.42
1:B:69:LYS:HE2	1:B:71:GLU:OE1	2.19	0.41
1:A:155:PHE:CD2	1:A:179:LYS:CD	3.03	0.41
1:A:210:GLU:O	1:A:213:LYS:HG2	2.21	0.41
1:B:14:GLU:CB	1:B:108:ILE:HG12	2.50	0.41
1:A:127:ASN:HB2	2:A:476:HOH:O	2.20	0.41
1:A:19:PRO:HB3	1:A:28:LEU:CD1	2.51	0.41
1:B:185:PHE:HE2	1:B:188:LEU:HB2	1.84	0.41
1:B:190:VAL:O	1:B:217:VAL:HA	2.20	0.41
1:B:241:VAL:O	1:B:244:VAL:HB	2.20	0.41
1:B:42:THR:C	1:B:43:LYS:HG3	2.39	0.41
1:A:19:PRO:HD2	1:A:103:LYS:O	2.20	0.41
1:A:39:PHE:CZ	1:A:87:ALA:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:HIS:HD2	2:B:365:HOH:O	2.02	0.41
1:A:129:PRO:O	1:A:131:ILE:HG12	2.21	0.41
1:B:315:VAL:HG12	1:B:317:ILE:HD12	2.02	0.41
1:B:204:LEU:O	1:B:208:TYR:N	2.44	0.41
1:B:220:VAL:HG12	2:B:415:HOH:O	2.20	0.41
1:B:269:GLY:O	1:B:273:VAL:HG23	2.21	0.41
1:A:27:HIS:O	1:A:31:ILE:HG12	2.20	0.41
1:B:19:PRO:HD2	1:B:103:LYS:O	2.21	0.41
1:B:314:LYS:HD3	2:B:394:HOH:O	2.20	0.41
1:A:124:GLU:C	2:A:475:HOH:O	2.60	0.40
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.93	0.40
1:B:175:GLU:HB3	1:B:179:LYS:CE	2.42	0.40
1:B:73:HIS:HE1	1:B:80:ARG:HB2	1.79	0.40

There are no symmetry-related clashes.

## 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	309/352 (88%)	291 (94%)	16 (5%)	2 (1%)	28	64
1	B	308/352 (88%)	289 (94%)	12 (4%)	7 (2%)	7	27
All	All	617/704 (88%)	580 (94%)	28 (4%)	9 (2%)	12	39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	61	VAL
1	B	220	VAL
1	B	138	GLU
1	B	171	GLU
1	B	155	PHE

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Mol	Chain	Res	Type
1	A	222	SER
1	A	62	ARG
1	B	67	VAL
1	B	154	ILE

### 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	270/300 (90%)	260 (96%)	10 (4%)	39	74
1	B	269/300 (90%)	247 (92%)	22 (8%)	13	37
All	All	539/600 (90%)	507 (94%)	32 (6%)	23	55

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	29	ARG
1	A	43	LYS
1	A	59	VAL
1	A	116	LEU
1	A	126	SER
1	A	128	ARG
1	A	171	GLU
1	A	207	ARG
1	A	257	LEU
1	B	29	ARG
1	B	42	THR
1	B	60	THR
1	B	62	ARG
1	B	85	ILE
1	B	105	LEU
1	B	142	VAL
1	B	151	VAL
1	B	154	ILE

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Mol	Chain	Res	Type
1	B	155	PHE
1	B	170	LYS
1	B	171	GLU
1	B	172	PHE
1	B	207	ARG
1	B	213	LYS
1	B	222	SER
1	B	223	VAL
1	B	233	LYS
1	B	243	GLU
1	B	257	LEU
1	B	341	ASN
1	B	343	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	73	HIS
1	A	77	ASN
1	A	148	GLN
1	A	198	ASN
1	A	214	ASN
1	B	27	HIS
1	B	73	HIS
1	B	77	ASN
1	B	98	ASN
1	B	115	GLN
1	B	127	ASN
1	B	198	ASN
1	B	278	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 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	317/352 (90%)	-0.43	11 (3%) 44 38	6, 27, 75, 119	0
1	B	316/352 (89%)	-0.11	20 (6%) 21 16	7, 35, 94, 137	0
All	All	633/704 (89%)	-0.27	31 (4%) 30 26	6, 31, 86, 137	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	THR	8.9
1	A	168	SER	6.3
1	B	43	LYS	5.9
1	B	148	GLN	5.6
1	B	92	SER	5.4
1	A	169	ARG	5.0
1	B	344	GLY	4.5
1	B	42	THR	4.5
1	B	61	VAL	4.2
1	B	195	PHE	4.1
1	A	88	GLY	4.0
1	A	195	PHE	4.0
1	A	59	VAL	3.6
1	B	154	ILE	3.1
1	B	181	GLU	3.1
1	A	219	ASP	2.8
1	B	150	GLY	2.8
1	A	60	THR	2.7
1	B	219	ASP	2.5
1	A	87	ALA	2.5
1	B	235	ARG	2.4
1	B	194	GLY	2.4
1	A	43	LYS	2.3
1	A	138	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	93	GLY	2.2
1	B	152	GLU	2.1
1	B	223	VAL	2.1
1	B	178	ALA	2.1
1	B	222	SER	2.1
1	B	207	ARG	2.0
1	B	206	GLU	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.