



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 04:23 AM EST

PDB ID : 1Y7P  
Title : 1.9 Å Crystal Structure of a Protein of Unknown Function AF1403 from *Archaeoglobus fulgidus*, Probable Metabolic Regulator  
Authors : Zhang, R.; Skarina, T.; Savchenko, A.; Edwards, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2004-12-09  
Resolution : 1.90 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

<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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

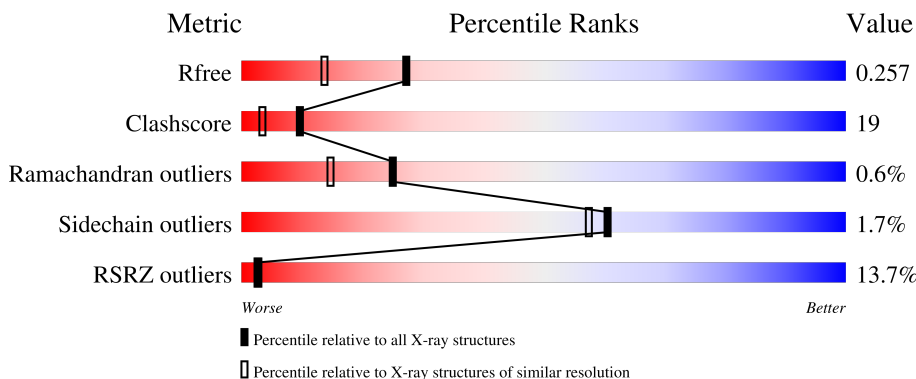
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	223	 16% 60% 33% • 5%
1	B	223	 2% 83% 14% •
1	C	223	 21% 56% 35% • 8%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5163 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.

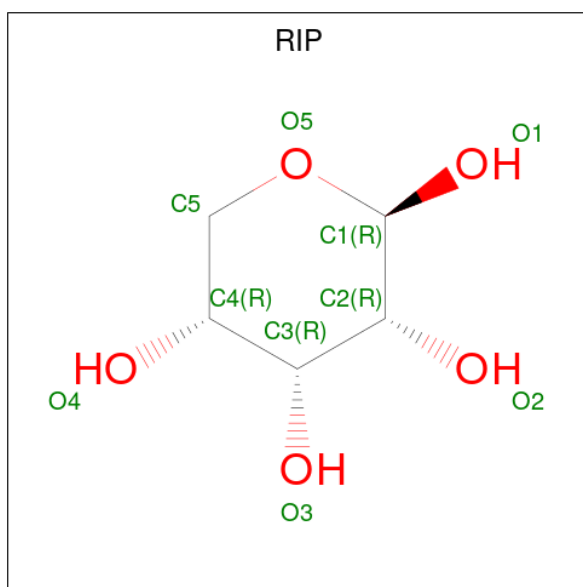
- Molecule 1 is a protein called Hypothetical protein AF1403.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	212	Total 1635	C 1040	N 286	O 304	S 5	0	0	0
1	B	217	Total 1668	C 1059	N 290	O 313	S 6	0	0	0
1	C	206	Total 1593	C 1013	N 279	O 296	S 5	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP O28869
A	0	HIS	-	cloning artifact	UNP O28869
A	220	GLY	-	cloning artifact	UNP O28869
A	221	LYS	-	cloning artifact	UNP O28869
B	-1	GLY	-	cloning artifact	UNP O28869
B	0	HIS	-	cloning artifact	UNP O28869
B	220	GLY	-	cloning artifact	UNP O28869
B	221	LYS	-	cloning artifact	UNP O28869
C	-1	GLY	-	cloning artifact	UNP O28869
C	0	HIS	-	cloning artifact	UNP O28869
C	220	GLY	-	cloning artifact	UNP O28869
C	221	LYS	-	cloning artifact	UNP O28869

- Molecule 2 is beta-D-ribose (three-letter code: RIP) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 5 5	0	0
2	B	1	Total C O 10 5 5	0	0
2	C	1	Total C O 10 5 5	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

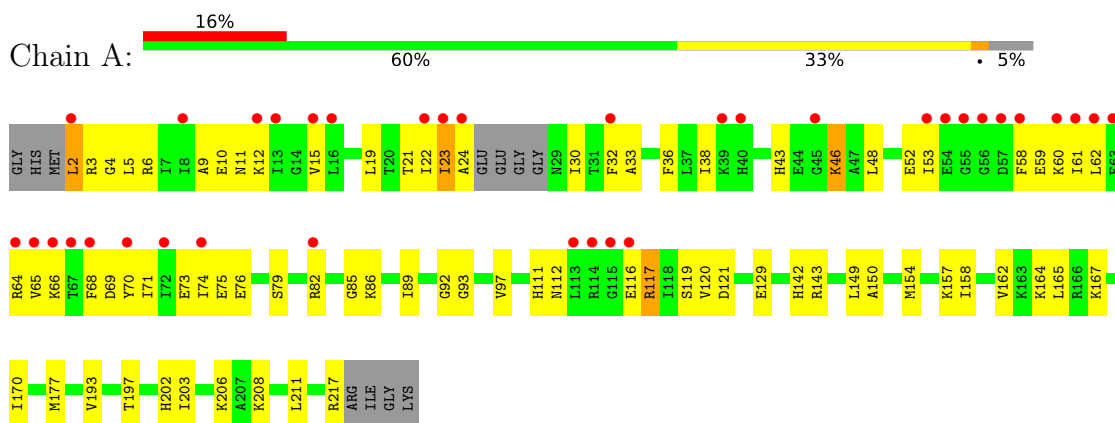
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	66	Total O 66 66	0	0
4	B	119	Total O 119 119	0	0
4	C	49	Total O 49 49	0	0

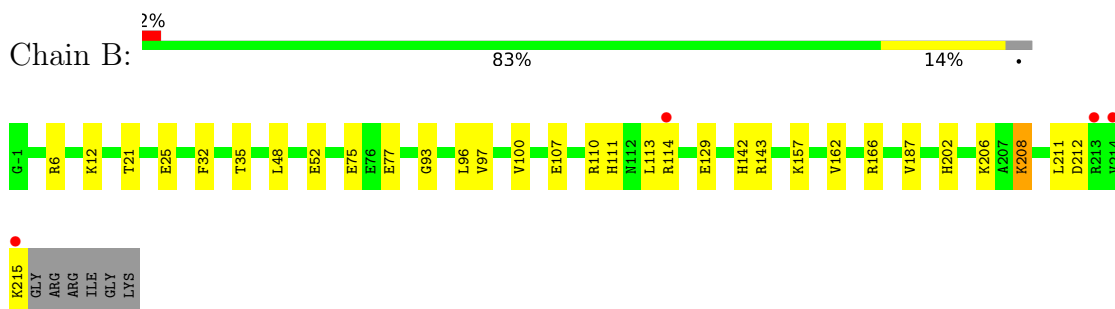
### 3 Residue-property plots [i](#)

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.

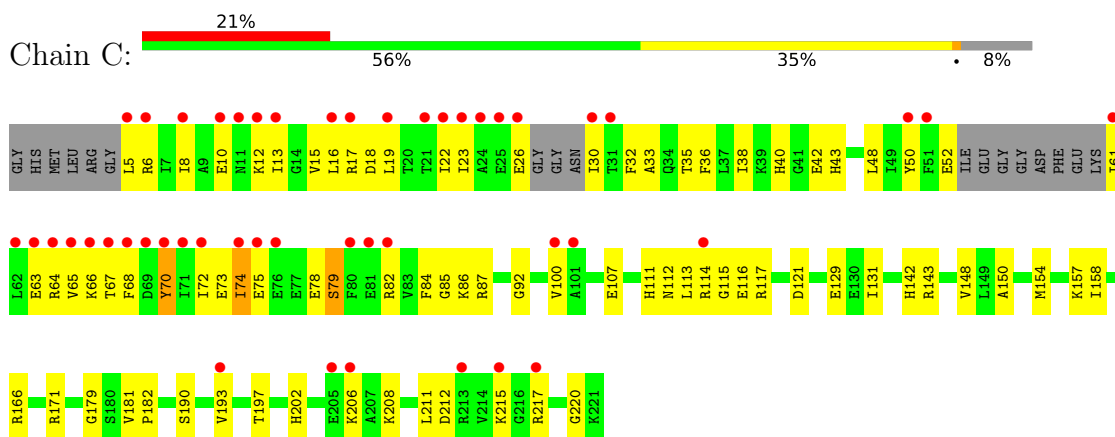
- Molecule 1: Hypothetical protein AF1403



- Molecule 1: Hypothetical protein AF1403



- Molecule 1: Hypothetical protein AF1403



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.71Å 95.71Å 167.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.34 – 1.90 36.34 – 1.90	Depositor EDS
% Data completeness (in resolution range)	87.4 (36.34-1.90) 92.0 (36.34-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 1.89Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.211 , 0.255 0.216 , 0.257	Depositor DCC
$R_{free}$ test set	5082 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.8	Xtrriage
Anisotropy	0.489	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 64.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5163	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.37	0/1652	0.61	0/2216
1	B	0.38	0/1687	0.63	0/2264
1	C	0.37	0/1608	0.59	0/2154
All	All	0.37	0/4947	0.61	0/6634

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 [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	1635	0	1706	79	0
1	B	1668	0	1731	26	0
1	C	1593	0	1669	95	0
2	A	10	0	10	4	0
2	B	10	0	10	0	0
2	C	10	0	10	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	66	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	119	0	0	3	1
4	C	49	0	0	8	0
All	All	5163	0	5136	195	1

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 19.

All (195) 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:202:HIS:HD2	1:B:211:LEU:H	1.08	0.99
1:C:154:MET:HE2	1:C:158:ILE:HD13	1.44	0.96
1:A:68:PHE:HB2	1:A:71:ILE:HD13	1.52	0.88
1:B:202:HIS:CD2	1:B:211:LEU:H	1.93	0.87
1:A:149:LEU:HB3	1:A:154:MET:HE1	1.58	0.86
1:A:202:HIS:HD2	1:A:211:LEU:H	1.25	0.83
1:B:212:ASP:HA	1:B:215:LYS:HE2	1.60	0.83
1:A:59:GLU:H	1:A:59:GLU:CD	1.82	0.83
1:A:121:ASP:HB3	2:C:4181:RIP:H4	1.60	0.82
1:C:202:HIS:HD2	1:C:211:LEU:H	1.27	0.82
1:C:114:ARG:HG3	1:C:206:LYS:HE2	1.62	0.82
1:C:131:ILE:HG21	1:C:154:MET:HE3	1.60	0.81
1:B:6:ARG:HH12	1:B:75:GLU:HB3	1.45	0.80
1:C:79:SER:OG	1:C:82:ARG:HG2	1.82	0.79
1:C:202:HIS:CD2	1:C:211:LEU:H	1.99	0.79
1:C:131:ILE:HG21	1:C:154:MET:CE	2.14	0.78
2:A:4182:RIP:H4	1:C:121:ASP:HB3	1.66	0.77
1:C:61:ILE:HA	4:C:525:HOH:O	1.82	0.77
1:A:59:GLU:HA	1:A:62:LEU:HD12	1.68	0.75
1:C:26:GLU:HB2	1:C:61:ILE:HD11	1.70	0.74
1:A:116:GLU:HB3	1:A:206:LYS:NZ	2.03	0.73
1:C:13:ILE:H	1:C:13:ILE:HD12	1.54	0.73
1:C:32:PHE:HB3	1:C:52:GLU:HB2	1.70	0.73
1:C:61:ILE:HG22	1:C:65:VAL:HG23	1.70	0.72
1:B:208:LYS:HD2	4:B:412:HOH:O	1.90	0.70
1:C:19:LEU:O	1:C:23:ILE:HG13	1.91	0.69
1:A:59:GLU:HA	1:A:62:LEU:CD1	2.21	0.69
1:A:202:HIS:CD2	1:A:211:LEU:H	2.08	0.68
1:A:149:LEU:HD13	1:A:154:MET:HE3	1.76	0.68
1:A:68:PHE:CB	1:A:71:ILE:HD13	2.23	0.67
1:B:48:LEU:HD12	4:B:464:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:O	1:A:19:LEU:HG	1.96	0.65
1:A:71:ILE:HG21	1:A:74:ILE:HD11	1.78	0.65
1:C:13:ILE:HD12	1:C:13:ILE:N	2.11	0.65
1:C:154:MET:HE1	1:C:158:ILE:HG21	1.79	0.65
1:A:58:PHE:O	1:A:62:LEU:HG	1.97	0.65
1:A:4:GLY:O	1:A:76:GLU:HG3	1.97	0.64
1:C:154:MET:CE	1:C:158:ILE:HG21	2.28	0.63
1:A:2:LEU:HD11	1:A:52:GLU:HB3	1.79	0.62
1:A:208:LYS:N	1:A:208:LYS:HD2	2.14	0.62
1:C:64:ARG:HG3	4:C:525:HOH:O	2.00	0.62
1:A:149:LEU:HB3	1:A:154:MET:CE	2.29	0.61
1:B:129:GLU:HG2	1:B:157:LYS:HD2	1.82	0.60
1:C:22:ILE:HG22	1:C:61:ILE:HG21	1.83	0.60
1:A:38:ILE:HB	1:A:43:HIS:O	2.02	0.60
1:A:22:ILE:HD11	1:A:68:PHE:CE2	2.37	0.59
1:A:6:ARG:HB3	1:A:6:ARG:NH1	2.18	0.59
1:A:12:LYS:HB2	1:A:15:VAL:HG23	1.84	0.59
1:C:16:LEU:HD21	1:C:35:THR:HG21	1.84	0.59
1:C:61:ILE:O	1:C:65:VAL:HG23	2.03	0.59
1:A:12:LYS:HB2	1:A:15:VAL:CG2	2.33	0.58
1:B:32:PHE:HB3	1:B:52:GLU:HB2	1.86	0.58
1:C:26:GLU:HB2	1:C:61:ILE:CD1	2.33	0.58
1:C:129:GLU:HG2	1:C:157:LYS:HD2	1.83	0.58
1:A:62:LEU:O	1:A:66:LYS:HG3	2.03	0.58
1:C:72:ILE:HG12	4:C:469:HOH:O	2.02	0.57
1:C:78:GLU:O	1:C:79:SER:HB3	2.05	0.57
1:A:33:ALA:HB3	1:C:35:THR:HG22	1.85	0.57
1:A:119:SER:HB2	4:A:402:HOH:O	2.05	0.57
1:C:18:ASP:O	1:C:22:ILE:HG13	2.05	0.57
1:A:23:ILE:HD13	1:A:53:ILE:HD11	1.85	0.56
1:A:10:GLU:OE2	1:A:70:TYR:HA	2.05	0.56
1:B:21:THR:O	1:B:25:GLU:HG3	2.06	0.56
1:A:60:LYS:O	1:A:64:ARG:HG3	2.05	0.56
1:C:12:LYS:O	1:C:15:VAL:HG23	2.06	0.56
1:C:74:ILE:O	1:C:74:ILE:HG23	2.06	0.56
1:A:6:ARG:HH12	1:A:75:GLU:HB3	1.71	0.56
1:B:142:HIS:HE1	4:B:506:HOH:O	1.88	0.55
1:C:12:LYS:HB2	1:C:15:VAL:CG2	2.36	0.55
1:B:6:ARG:HB3	1:B:6:ARG:HH11	1.72	0.55
1:C:78:GLU:O	1:C:79:SER:CB	2.54	0.55
1:B:107:GLU:O	1:B:111:HIS:HD2	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ILE:O	1:A:75:GLU:HB2	2.07	0.54
1:A:32:PHE:HD1	1:C:36:PHE:HB3	1.73	0.54
1:C:63:GLU:O	1:C:67:THR:HG23	2.07	0.54
1:A:3:ARG:HH11	1:A:3:ARG:HG3	1.73	0.54
1:C:171:ARG:HG2	1:C:171:ARG:HH11	1.73	0.53
1:B:142:HIS:CD2	1:B:143:ARG:HE	2.27	0.53
1:A:43:HIS:HE1	1:A:73:GLU:OE2	1.91	0.53
1:A:116:GLU:HB3	1:A:206:LYS:HZ2	1.69	0.53
1:C:6:ARG:HB3	1:C:75:GLU:O	2.08	0.53
1:C:84:PHE:HB3	2:C:4181:RIP:H1	1.90	0.53
1:C:38:ILE:H	1:C:38:ILE:HD12	1.72	0.52
1:C:61:ILE:HG23	1:C:64:ARG:HB2	1.91	0.52
1:C:38:ILE:HD12	1:C:38:ILE:N	2.25	0.52
1:A:15:VAL:HG13	1:A:70:TYR:CE1	2.44	0.52
1:A:5:LEU:HD13	1:A:58:PHE:CZ	2.44	0.52
1:C:166:ARG:HD2	4:C:433:HOH:O	2.09	0.52
1:C:217:ARG:HG2	1:C:217:ARG:HH11	1.75	0.52
1:A:33:ALA:HB3	1:C:35:THR:CG2	2.41	0.51
1:C:61:ILE:HG22	1:C:61:ILE:O	2.11	0.51
1:B:111:HIS:O	1:B:206:LYS:NZ	2.42	0.51
1:C:10:GLU:HG2	4:C:469:HOH:O	2.10	0.51
1:A:59:GLU:CD	1:A:59:GLU:N	2.60	0.51
1:C:166:ARG:NH2	4:C:433:HOH:O	2.43	0.51
1:C:86:LYS:HZ1	1:C:116:GLU:CD	2.15	0.50
1:C:114:ARG:O	1:C:116:GLU:N	2.37	0.50
1:C:114:ARG:HE	1:C:206:LYS:HD2	1.76	0.50
1:C:12:LYS:HB2	1:C:15:VAL:HG22	1.94	0.49
1:A:61:ILE:O	1:A:65:VAL:HG23	2.13	0.49
1:A:154:MET:HE2	1:A:177:MET:SD	2.53	0.49
1:B:162:VAL:O	1:B:166:ARG:HG3	2.13	0.49
1:B:6:ARG:HB2	1:B:77:GLU:HG3	1.94	0.49
1:C:26:GLU:HG3	1:C:61:ILE:HG12	1.94	0.48
1:A:21:THR:HA	1:C:17:ARG:HG3	1.94	0.48
1:C:13:ILE:H	1:C:13:ILE:CD1	2.22	0.48
1:C:38:ILE:HD11	1:C:48:LEU:HB2	1.95	0.48
1:C:112:ASN:HA	1:C:116:GLU:O	2.13	0.48
1:B:12:LYS:HA	1:B:12:LYS:HE2	1.95	0.48
1:C:111:HIS:O	1:C:116:GLU:HB2	2.13	0.48
1:C:66:LYS:C	1:C:68:PHE:H	2.16	0.48
1:A:165:LEU:HG	1:A:170:ILE:HB	1.96	0.48
1:A:116:GLU:HB3	1:A:206:LYS:HZ1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:VAL:O	1:A:197:THR:HG23	2.13	0.48
1:A:2:LEU:HD13	1:A:3:ARG:N	2.29	0.47
1:A:19:LEU:O	1:A:23:ILE:HG13	2.14	0.47
1:C:6:ARG:HD3	4:C:484:HOH:O	2.14	0.47
1:B:6:ARG:NH1	1:B:75:GLU:HB3	2.21	0.47
1:A:5:LEU:HB2	1:A:58:PHE:HE1	1.80	0.47
1:A:3:ARG:HG3	1:A:3:ARG:NH1	2.30	0.47
1:B:113:LEU:HG	1:B:114:ARG:HG3	1.96	0.47
1:C:142:HIS:O	1:C:143:ARG:HB2	2.15	0.47
1:A:89:ILE:HG23	2:C:4181:RIP:O4	2.15	0.47
1:A:92:GLY:HA3	1:A:150:ALA:O	2.14	0.47
1:A:65:VAL:HG12	1:A:71:ILE:HG12	1.97	0.46
1:C:100:VAL:HG11	1:C:148:VAL:HG11	1.98	0.46
1:A:70:TYR:CD1	1:A:71:ILE:HD12	2.51	0.46
1:C:61:ILE:CG2	1:C:64:ARG:HB2	2.46	0.46
1:C:190:SER:HB3	1:C:220:GLY:HA3	1.98	0.46
1:A:5:LEU:HB2	1:A:58:PHE:CE1	2.51	0.46
1:A:32:PHE:HB3	1:A:52:GLU:HB2	1.98	0.46
1:A:79:SER:OG	1:A:82:ARG:HG2	2.16	0.46
1:A:93:GLY:O	1:A:97:VAL:HG23	2.16	0.46
1:C:193:VAL:O	1:C:197:THR:HG23	2.16	0.46
1:B:93:GLY:O	1:B:97:VAL:HG23	2.16	0.46
1:C:131:ILE:CG2	1:C:154:MET:HE3	2.41	0.46
1:C:68:PHE:HB3	1:C:70:TYR:CE1	2.50	0.45
1:C:114:ARG:NE	1:C:206:LYS:HD2	2.31	0.45
1:A:23:ILE:HD12	1:A:30:ILE:HD11	1.99	0.45
2:A:4182:RIP:C4	1:C:121:ASP:HB3	2.41	0.45
1:C:85:GLY:HA3	1:C:117:ARG:O	2.17	0.45
1:C:113:LEU:O	1:C:113:LEU:HG	2.16	0.45
2:A:4182:RIP:H3	1:C:87:ARG:NH2	2.31	0.45
1:A:85:GLY:HA3	1:A:117:ARG:HB3	1.99	0.45
1:B:6:ARG:HB3	1:B:6:ARG:NH1	2.30	0.45
1:C:107:GLU:O	1:C:111:HIS:HD2	2.00	0.45
1:A:9:ALA:O	1:A:46:LYS:HG2	2.18	0.44
1:A:111:HIS:O	1:A:206:LYS:HE2	2.17	0.44
1:A:142:HIS:O	1:A:143:ARG:HB2	2.18	0.44
1:B:107:GLU:OE2	1:B:110:ARG:NH2	2.50	0.44
1:B:129:GLU:HG2	1:B:157:LYS:CD	2.47	0.44
1:C:61:ILE:HG22	1:C:65:VAL:CG2	2.45	0.44
1:C:5:LEU:N	1:C:50:TYR:HE1	2.15	0.44
1:C:65:VAL:O	1:C:68:PHE:HD2	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LYS:HD2	1:A:208:LYS:H	1.82	0.43
1:C:16:LEU:HD12	1:C:16:LEU:N	2.33	0.43
1:C:166:ARG:HH21	1:C:166:ARG:HB3	1.82	0.43
1:C:212:ASP:HA	1:C:215:LYS:HE3	1.99	0.43
1:A:164:LYS:O	1:A:167:LYS:HG2	2.18	0.43
1:A:217:ARG:HD3	1:A:217:ARG:HA	1.72	0.43
1:C:42:GLU:HG3	1:C:43:HIS:N	2.32	0.43
1:A:59:GLU:O	1:A:62:LEU:HB2	2.18	0.43
1:A:120:VAL:N	4:A:402:HOH:O	2.50	0.43
1:A:112:ASN:HA	1:A:116:GLU:O	2.19	0.43
1:B:35:THR:HA	1:B:48:LEU:O	2.19	0.42
1:C:8:ILE:HB	1:C:73:GLU:HB2	2.02	0.42
1:C:166:ARG:CZ	4:C:433:HOH:O	2.67	0.42
1:A:48:LEU:C	1:A:48:LEU:HD13	2.40	0.42
1:C:5:LEU:O	1:C:50:TYR:HD1	2.03	0.42
1:C:154:MET:HB3	1:C:181:VAL:HG21	2.00	0.42
1:C:42:GLU:HG3	1:C:43:HIS:CD2	2.54	0.42
1:C:6:ARG:O	1:C:74:ILE:HA	2.19	0.42
1:C:92:GLY:HA3	1:C:150:ALA:O	2.19	0.42
1:A:129:GLU:HG2	1:A:157:LYS:HD2	2.01	0.42
1:A:23:ILE:CD1	1:A:30:ILE:HD11	2.50	0.42
1:C:212:ASP:HB3	1:C:215:LYS:HE3	2.01	0.42
1:A:36:PHE:HB3	1:C:32:PHE:HD1	1.85	0.42
1:C:30:ILE:CG2	1:C:33:ALA:HB2	2.50	0.42
1:C:131:ILE:HG21	1:C:154:MET:HE2	1.98	0.42
1:C:202:HIS:HD2	1:C:211:LEU:N	2.07	0.41
1:A:142:HIS:CD2	1:A:143:ARG:HE	2.38	0.41
1:A:154:MET:HE2	1:A:154:MET:HB2	1.92	0.41
1:A:86:LYS:HD3	1:A:203:ILE:HG23	2.01	0.41
1:C:8:ILE:HD13	1:C:43:HIS:CD2	2.56	0.41
1:C:117:ARG:HD3	1:C:117:ARG:HA	1.66	0.41
1:C:179:GLY:O	1:C:182:PRO:HD2	2.20	0.41
1:A:22:ILE:HD11	1:A:68:PHE:HE2	1.81	0.41
1:A:158:ILE:O	1:A:162:VAL:HG23	2.21	0.41
1:B:96:LEU:O	1:B:100:VAL:HG23	2.21	0.41
1:C:70:TYR:C	1:C:70:TYR:CD1	2.93	0.41
1:C:87:ARG:HG2	2:C:4181:RIP:O1	2.21	0.41
1:A:21:THR:O	1:A:24:ALA:HB3	2.21	0.41
1:A:121:ASP:OD1	2:A:4182:RIP:H4	2.20	0.41
1:C:154:MET:HE2	1:C:158:ILE:HG21	2.00	0.41
1:B:187:VAL:HG21	1:B:211:LEU:HD22	2.02	0.40

All (1) 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)
4:B:310:HOH:O	4:B:310:HOH:O[7_555]	1.38	0.82

## 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	208/223 (93%)	197 (95%)	10 (5%)	1 (0%)	29	18
1	B	215/223 (96%)	210 (98%)	5 (2%)	0	100	100
1	C	200/223 (90%)	183 (92%)	14 (7%)	3 (2%)	10	3
All	All	623/669 (93%)	590 (95%)	29 (5%)	4 (1%)	25	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	74	ILE
1	C	79	SER
1	C	115	GLY
1	A	23	ILE

### 5.3.2 Protein sidechains [i](#)

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	174/181 (96%)	169 (97%)	5 (3%)	42	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	177/181 (98%)	176 (99%)	1 (1%)	86	87
1	C	170/181 (94%)	167 (98%)	3 (2%)	59	55
All	All	521/543 (96%)	512 (98%)	9 (2%)	60	57

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	11	ASN
1	A	46	LYS
1	A	69	ASP
1	A	117	ARG
1	B	208	LYS
1	C	40	HIS
1	C	70	TYR
1	C	208	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	40	HIS
1	A	43	HIS
1	A	142	HIS
1	A	202	HIS
1	B	11	ASN
1	B	99	GLN
1	B	142	HIS
1	B	202	HIS
1	C	11	ASN
1	C	40	HIS
1	C	43	HIS
1	C	202	HIS

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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
2	RIP	B	4183	-	10,10,10	1.27	1 (10%)	14,14,14	0.77	0
2	RIP	C	4181	-	10,10,10	1.31	1 (10%)	14,14,14	0.68	0
2	RIP	A	4182	-	10,10,10	1.36	2 (20%)	14,14,14	0.71	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
2	RIP	B	4183	-	-	-	0/1/1/1
2	RIP	C	4181	-	-	-	0/1/1/1
2	RIP	A	4182	-	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4182	RIP	O5-C1	3.01	1.47	1.43
2	C	4181	RIP	O5-C1	2.80	1.47	1.43
2	B	4183	RIP	O5-C1	2.05	1.45	1.43
2	A	4182	RIP	O5-C5	2.05	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4181	RIP	4	0
2	A	4182	RIP	4	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	212/223 (95%)	0.93	36 (16%) <b>1</b> <b>1</b>	18, 32, 75, 81	0
1	B	217/223 (97%)	0.03	4 (1%) 68 71	16, 24, 42, 67	0
1	C	206/223 (92%)	1.21	47 (22%) <b>0</b> <b>0</b>	18, 36, 76, 80	0
All	All	635/669 (94%)	0.71	87 (13%) <b>3</b> <b>3</b>	16, 28, 75, 81	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	65	VAL	11.0
1	A	58	PHE	9.5
1	A	65	VAL	9.3
1	C	24	ALA	8.2
1	C	67	THR	6.7
1	C	75	GLU	6.5
1	A	114	ARG	5.9
1	C	13	ILE	5.8
1	C	61	ILE	5.8
1	B	114	ARG	5.8
1	C	62	LEU	5.7
1	C	70	TYR	5.5
1	C	68	PHE	5.3
1	C	12	LYS	5.0
1	A	115	GLY	5.0
1	C	63	GLU	4.9
1	A	62	LEU	4.9
1	A	57	ASP	4.9
1	C	25	GLU	4.9
1	A	56	GLY	4.5
1	C	69	ASP	4.5
1	A	24	ALA	4.5
1	C	22	ILE	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	70	TYR	4.2
1	A	23	ILE	4.1
1	C	16	LEU	4.1
1	A	61	ILE	4.0
1	C	23	ILE	4.0
1	A	60	LYS	3.9
1	A	53	ILE	3.8
1	C	64	ARG	3.7
1	C	114	ARG	3.7
1	A	16	LEU	3.7
1	A	45	GLY	3.6
1	A	54	GLU	3.5
1	C	26	GLU	3.5
1	C	74	ILE	3.4
1	A	2	LEU	3.4
1	A	82	ARG	3.2
1	C	217	ARG	3.1
1	A	68	PHE	3.1
1	A	39	LYS	3.0
1	C	21	THR	2.9
1	B	214	VAL	2.9
1	C	30	ILE	2.8
1	C	76	GLU	2.8
1	C	50	TYR	2.8
1	A	22	ILE	2.7
1	C	82	ARG	2.7
1	A	63	GLU	2.7
1	A	67	THR	2.7
1	C	17	ARG	2.7
1	C	71	ILE	2.6
1	C	72	ILE	2.6
1	A	72	ILE	2.6
1	C	5	LEU	2.5
1	C	8	ILE	2.4
1	A	8	ILE	2.4
1	A	55	GLY	2.4
1	C	31	THR	2.4
1	A	74	ILE	2.4
1	C	100	VAL	2.4
1	C	80	PHE	2.4
1	B	213	ARG	2.3
1	C	19	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	213	ARG	2.3
1	C	81	GLU	2.3
1	C	206	LYS	2.3
1	A	66	LYS	2.3
1	C	101	ALA	2.3
1	A	13	ILE	2.2
1	A	113	LEU	2.2
1	B	215	LYS	2.2
1	A	64	ARG	2.2
1	C	51	PHE	2.2
1	C	205	GLU	2.2
1	A	116	GLU	2.2
1	C	11	ASN	2.1
1	A	40	HIS	2.1
1	A	12	LYS	2.1
1	C	66	LYS	2.1
1	A	15	VAL	2.1
1	C	193	VAL	2.1
1	C	215	LYS	2.1
1	C	6	ARG	2.0
1	A	32	PHE	2.0
1	C	10	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 monosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	RIP	A	4182	10/10	0.73	0.34	65,67,69,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	RIP	C	4181	10/10	0.77	0.37	64,65,68,70	0
2	RIP	B	4183	10/10	0.80	0.32	41,43,44,46	0
3	ZN	C	302	1/1	0.97	0.06	47,47,47,47	0
3	ZN	A	301	1/1	0.99	0.07	44,44,44,44	0
3	ZN	B	303	1/1	1.00	0.06	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.