



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2024 – 02:41 PM EDT

PDB ID : 2PCR  
Title : Crystal structure of Myo-inositol-1(or 4)-monophosphatase (aq\_1983) from Aquifex Aeolicus VF5  
Authors : Jeyakanthan, J.; Gayathri, D.; Velmurugan, D.; Agari, Y.; Bessho, Y.; Ellis, M.J.; Antonyuk, S.V.; Strange, R.W.; Hasnain, S.S.; Ebihara, A.; Kuramitsu, S.; Shinkai, A.; Shiro, Y.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2007-03-30  
Resolution : 2.60 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)

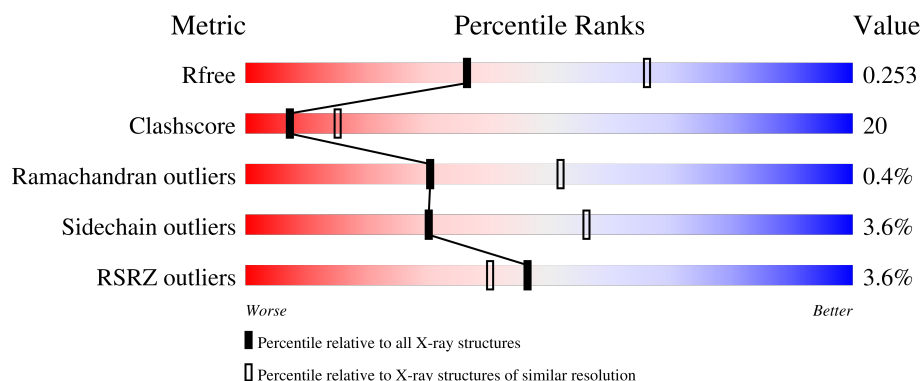
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	264	<div> <div>2%</div> <div> <div></div> <div>56%</div> <div>32%</div> <div>• 10%</div> </div> </div>
1	B	264	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>• 9%</div> </div> </div>
1	C	264	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>28%</div> <div>• 9%</div> </div> </div>
1	D	264	<div> <div>5%</div> <div> <div></div> <div>52%</div> <div>35%</div> <div>• 9%</div> </div> </div>

Validation Pipeline (wwPDB-VP) : 2.39

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7854 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 Inositol-1-monophosphatase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	Se	0	0	0
			1871	1224	303	337	1	6			
1	B	241	Total	C	N	O	S	Se	0	0	0
			1895	1239	306	342	1	7			
1	C	241	Total	C	N	O	S	Se	0	0	0
			1891	1238	303	342	1	7			
1	D	240	Total	C	N	O	S	Se	0	0	0
			1885	1237	302	339	1	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP O67791
A	72	MSE	MET	modified residue	UNP O67791
A	184	MSE	MET	modified residue	UNP O67791
A	196	MSE	MET	modified residue	UNP O67791
A	205	MSE	MET	modified residue	UNP O67791
A	206	MSE	MET	modified residue	UNP O67791
A	210	MSE	MET	modified residue	UNP O67791
A	260	MSE	MET	modified residue	UNP O67791
B	1	MSE	MET	modified residue	UNP O67791
B	72	MSE	MET	modified residue	UNP O67791
B	184	MSE	MET	modified residue	UNP O67791
B	196	MSE	MET	modified residue	UNP O67791
B	205	MSE	MET	modified residue	UNP O67791
B	206	MSE	MET	modified residue	UNP O67791
B	210	MSE	MET	modified residue	UNP O67791
B	260	MSE	MET	modified residue	UNP O67791
C	1	MSE	MET	modified residue	UNP O67791
C	72	MSE	MET	modified residue	UNP O67791
C	184	MSE	MET	modified residue	UNP O67791
C	196	MSE	MET	modified residue	UNP O67791
C	205	MSE	MET	modified residue	UNP O67791

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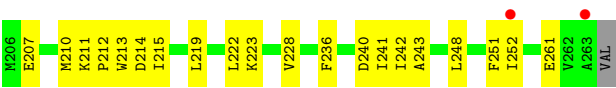
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Chain	Residue	Modelled	Actual	Comment	Reference
C	206	MSE	MET	modified residue	UNP O67791
C	210	MSE	MET	modified residue	UNP O67791
C	260	MSE	MET	modified residue	UNP O67791
D	1	MSE	MET	modified residue	UNP O67791
D	72	MSE	MET	modified residue	UNP O67791
D	184	MSE	MET	modified residue	UNP O67791
D	196	MSE	MET	modified residue	UNP O67791
D	205	MSE	MET	modified residue	UNP O67791
D	206	MSE	MET	modified residue	UNP O67791
D	210	MSE	MET	modified residue	UNP O67791
D	260	MSE	MET	modified residue	UNP O67791

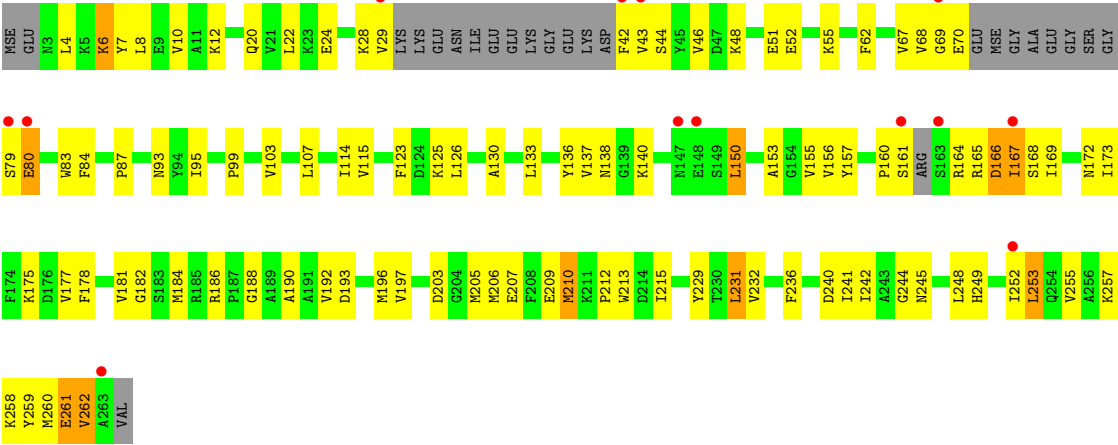
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	77	Total O 77 77	0	0
2	B	82	Total O 82 82	0	0
2	C	84	Total O 84 84	0	0
2	D	69	Total O 69 69	0	0





● Molecule 1: Inositol-1-monophosphatase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.00Å 68.16Å 96.94Å 90.00° 97.86° 90.00°	Depositor
Resolution (Å)	36.42 – 2.60 36.42 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.8 (36.42-2.60) 98.0 (36.42-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.31 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.190 , 0.247 0.197 , 0.253	Depositor DCC
$R_{free}$ test set	1658 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.773	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.0	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	0.94	EDS
Total number of atoms	7854	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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](#)

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	0.40	0/1907	0.65	1/2559 (0.0%)
1	B	0.37	0/1931	0.62	0/2591
1	C	0.39	0/1926	0.62	0/2584
1	D	0.37	0/1921	0.64	2/2578 (0.1%)
All	All	0.38	0/7685	0.63	3/10312 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	GLY	N-CA-C	6.35	128.98	113.10
1	D	80	GLU	CB-CA-C	-6.12	98.17	110.40
1	D	261	GLU	N-CA-C	5.46	125.73	111.00

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	1871	0	1885	96	0
1	B	1895	0	1912	64	0
1	C	1891	0	1907	63	0
1	D	1885	0	1898	107	0
2	A	77	0	0	3	0
2	B	82	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	84	0	0	5	0
2	D	69	0	0	0	0
All	All	7854	0	7602	308	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 20.

All (308) 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:D:203:ASP:HB2	1:D:248:LEU:HD12	1.29	1.10
1:A:262:VAL:HG12	1:A:263:ALA:H	1.19	1.06
1:D:261:GLU:O	1:D:261:GLU:HG2	1.54	1.05
1:A:205:MSE:HE2	1:A:207:GLU:HB2	1.37	1.03
1:B:167:ILE:HD12	1:B:167:ILE:H	1.25	1.00
1:D:207:GLU:HG2	1:D:210:MSE:SE	2.20	0.91
1:A:55:LYS:HG2	1:A:67:VAL:HG11	1.53	0.90
1:A:160:PRO:HG2	1:A:163:SER:HB3	1.53	0.87
1:D:203:ASP:CB	1:D:248:LEU:HD12	2.05	0.84
1:A:194:LEU:HD13	1:A:205:MSE:SE	2.30	0.82
1:B:1:MSE:HE2	1:B:109:LYS:HD2	1.63	0.81
1:B:1:MSE:CE	1:B:109:LYS:HD2	2.10	0.80
1:A:149:SER:HB3	1:A:152:HIS:HD2	1.46	0.80
1:B:151:LYS:HG3	1:B:152:HIS:HD2	1.47	0.79
1:A:262:VAL:HG12	1:A:263:ALA:N	1.98	0.79
1:A:175:LYS:HD2	1:D:167:ILE:HD12	1.65	0.79
1:D:203:ASP:HB2	1:D:248:LEU:CD1	2.13	0.78
1:D:212:PRO:HG3	1:D:236:PHE:HA	1.66	0.76
1:A:185:ARG:HE	1:D:93:ASN:HD21	1.33	0.76
1:C:194:LEU:HD13	1:C:205:MSE:SE	2.35	0.76
1:A:206:MSE:HG2	1:A:252:ILE:HG21	1.66	0.76
1:B:183:SER:HB3	1:C:92:LYS:HG2	1.68	0.76
1:C:157:TYR:CD2	1:C:184:MSE:HE2	2.23	0.74
1:D:69:GLY:HA2	1:D:213:TRP:CE3	2.23	0.74
1:A:161:SER:HA	1:D:178:PHE:CE2	2.23	0.73
1:B:232:VAL:HB	1:B:240:ASP:HB2	1.69	0.73
1:D:153:ALA:HB1	1:D:248:LEU:HD11	1.70	0.72
1:A:150:LEU:HD23	1:A:181:VAL:HG12	1.71	0.72
1:B:222:LEU:HD21	1:B:243:ALA:HB1	1.72	0.72
1:B:205:MSE:HE3	1:B:207:GLU:CG	2.20	0.72
1:D:232:VAL:HG11	1:D:260:MSE:HE2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:LEU:HD21	1:C:243:ALA:HB1	1.74	0.70
1:C:228:VAL:HG22	2:C:314:HOH:O	1.91	0.70
1:A:79:SER:O	1:A:80:GLU:HB3	1.90	0.70
1:B:1:MSE:HE1	1:B:114:ILE:HD13	1.74	0.69
1:C:207:GLU:HG3	1:C:210:MSE:SE	2.42	0.69
1:D:248:LEU:O	1:D:252:ILE:HG12	1.92	0.69
1:D:126:LEU:H	1:D:138:ASN:ND2	1.91	0.69
1:B:69:GLY:O	1:B:70:GLU:HG2	1.92	0.69
1:D:80:GLU:O	1:D:80:GLU:HG3	1.91	0.69
1:D:107:LEU:HB3	1:D:115:VAL:HB	1.74	0.69
1:B:25:ASN:HA	1:B:28:LYS:HD3	1.74	0.68
1:B:194:LEU:HD13	1:B:205:MSE:SE	2.44	0.67
1:B:210:MSE:HE2	1:B:210:MSE:HA	1.77	0.66
1:A:206:MSE:CG	1:A:252:ILE:HD13	2.26	0.66
1:A:163:SER:HB2	1:A:209:GLU:OE2	1.96	0.65
1:B:181:VAL:HG12	1:B:183:SER:H	1.61	0.65
1:C:205:MSE:CE	1:C:207:GLU:HB2	2.27	0.65
1:D:257:LYS:HE2	1:D:262:VAL:HG13	1.78	0.65
1:C:119:TYR:O	1:C:121:PRO:HD3	1.96	0.64
1:A:70:GLU:HB2	1:A:213:TRP:CZ2	2.32	0.64
1:D:253:LEU:HD22	1:D:257:LYS:HE3	1.80	0.64
1:D:206:MSE:CE	1:D:252:ILE:HB	2.28	0.64
1:A:171:LEU:O	1:A:175:LYS:HG3	1.98	0.64
1:A:137:VAL:HG13	1:A:137:VAL:O	1.98	0.63
1:C:137:VAL:HG13	1:C:137:VAL:O	1.98	0.63
1:D:205:MSE:HE1	1:D:241:ILE:HG23	1.80	0.63
1:D:229:TYR:HB2	1:D:241:ILE:HD11	1.79	0.62
1:A:197:VAL:HG11	1:A:244:GLY:HA2	1.82	0.62
1:A:178:PHE:HE1	1:D:186:ARG:HH22	1.48	0.62
1:A:185:ARG:NE	1:D:93:ASN:HD21	1.99	0.61
1:B:205:MSE:HE3	1:B:207:GLU:HG2	1.82	0.61
1:D:212:PRO:CG	1:D:236:PHE:HA	2.29	0.61
1:A:262:VAL:CG1	1:A:263:ALA:H	2.04	0.61
1:B:92:LYS:HD3	1:C:183:SER:HB3	1.82	0.61
1:C:100:ILE:HD13	1:C:187:PRO:HB3	1.82	0.61
1:A:164:ARG:HH21	1:A:209:GLU:HG2	1.67	0.60
1:D:206:MSE:HE3	1:D:252:ILE:HB	1.83	0.60
1:B:102:ALA:HB2	1:B:120:LEU:CD2	2.31	0.60
1:D:255:VAL:O	1:D:258:LYS:HB3	2.02	0.60
1:C:222:LEU:CD2	1:C:243:ALA:HB1	2.32	0.59
1:D:22:LEU:HD22	1:D:103:VAL:HG23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:GLY:O	1:D:70:GLU:HB3	2.02	0.59
1:A:206:MSE:HG3	1:A:252:ILE:HD13	1.84	0.59
1:A:149:SER:HB3	1:A:152:HIS:CD2	2.33	0.59
1:A:222:LEU:CD2	1:A:243:ALA:HB1	2.33	0.58
1:B:256:ALA:O	1:B:260:MSE:HG2	2.03	0.58
1:C:205:MSE:HE2	1:C:207:GLU:HB2	1.83	0.58
1:C:20:GLN:O	1:C:24:GLU:HG2	2.02	0.58
1:D:43:VAL:HG23	1:D:44:SER:H	1.68	0.58
1:A:206:MSE:HG2	1:A:252:ILE:CG2	2.34	0.58
1:C:1:MSE:SE	1:C:4:LEU:HD13	2.54	0.58
1:B:151:LYS:HG3	1:B:152:HIS:CD2	2.33	0.58
1:C:261:GLU:CD	1:C:261:GLU:H	2.07	0.58
1:B:193:ASP:O	1:B:197:VAL:HG23	2.04	0.58
1:A:212:PRO:HB3	1:A:236:PHE:HA	1.85	0.58
1:D:177:VAL:HG22	1:D:252:ILE:HG22	1.86	0.57
1:C:1:MSE:HG3	1:C:1:MSE:O	2.05	0.57
1:C:185:ARG:NH2	2:C:318:HOH:O	2.37	0.57
1:D:156:VAL:CG2	1:D:205:MSE:HB3	2.34	0.57
1:C:261:GLU:CD	1:C:261:GLU:N	2.57	0.57
1:A:178:PHE:CE2	1:D:161:SER:HA	2.40	0.57
1:D:137:VAL:O	1:D:137:VAL:HG13	2.04	0.57
1:D:165:ARG:NH2	1:D:260:MSE:HE3	2.20	0.57
1:B:205:MSE:HE3	1:B:207:GLU:HG3	1.86	0.57
1:D:55:LYS:HG3	1:D:67:VAL:HG21	1.87	0.57
1:B:23:LYS:NZ	1:B:119:TYR:OH	2.39	0.56
1:A:69:GLY:HA2	1:A:213:TRP:CE3	2.40	0.56
1:B:165:ARG:HH22	1:B:240:ASP:CG	2.09	0.56
1:B:157:TYR:CD1	1:B:184:MSE:HE2	2.41	0.56
1:A:114:ILE:HG13	1:A:115:VAL:HG23	1.87	0.56
1:C:261:GLU:HG2	2:C:341:HOH:O	2.05	0.56
1:A:172:ASN:HA	1:A:175:LYS:HE2	1.88	0.56
1:D:6:LYS:HD2	1:D:6:LYS:N	2.18	0.56
1:D:231:LEU:CD1	1:D:241:ILE:HD13	2.36	0.56
1:C:50:SER:O	1:C:54:ILE:HG13	2.06	0.56
1:C:20:GLN:HA	1:C:23:LYS:HD3	1.87	0.55
1:D:197:VAL:HG11	1:D:244:GLY:HA2	1.88	0.55
1:A:172:ASN:HD22	1:A:175:LYS:HE2	1.72	0.55
1:D:80:GLU:O	1:D:80:GLU:CG	2.54	0.55
1:A:149:SER:CB	1:A:152:HIS:HD2	2.18	0.55
1:B:222:LEU:CD2	1:B:243:ALA:HB1	2.37	0.54
1:C:20:GLN:OE1	1:C:23:LYS:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:HIS:O	1:D:253:LEU:HB2	2.07	0.54
1:A:196:MSE:HE2	2:A:326:HOH:O	2.06	0.54
1:B:261:GLU:H	1:B:261:GLU:CD	2.11	0.54
1:A:82:ARG:O	1:A:107:LEU:HD12	2.08	0.54
1:A:179:TYR:CE2	1:D:167:ILE:HD13	2.43	0.54
1:A:51:GLU:HB3	1:A:87:PRO:HB3	1.89	0.54
1:A:222:LEU:HD22	1:A:243:ALA:HB1	1.91	0.53
1:B:102:ALA:HB2	1:B:120:LEU:HD23	1.91	0.53
1:D:155:VAL:O	1:D:184:MSE:HA	2.09	0.53
1:A:206:MSE:HG2	1:A:252:ILE:HD13	1.89	0.53
1:D:55:LYS:HE3	1:D:67:VAL:HB	1.91	0.53
1:C:215:ILE:O	1:C:219:LEU:HB2	2.08	0.53
1:C:210:MSE:HE3	1:C:214:ASP:HB3	1.91	0.53
1:D:20:GLN:O	1:D:24:GLU:HG2	2.09	0.52
1:A:242:ILE:HG23	1:A:252:ILE:CG2	2.40	0.52
1:B:161:SER:HA	1:C:178:PHE:CE2	2.45	0.52
1:A:91:THR:O	1:A:95:ILE:HG13	2.10	0.52
1:A:164:ARG:NH2	1:A:209:GLU:HG2	2.23	0.51
1:A:156:VAL:HA	1:A:185:ARG:O	2.11	0.51
1:A:6:LYS:HE3	1:A:62:PHE:HE1	1.75	0.51
1:A:156:VAL:O	1:A:205:MSE:HA	2.10	0.51
1:A:149:SER:OG	1:A:151:LYS:HG2	2.11	0.51
1:A:80:GLU:O	1:A:80:GLU:HG2	2.11	0.51
1:D:43:VAL:HG23	1:D:44:SER:N	2.24	0.51
1:A:160:PRO:HG2	1:A:163:SER:CB	2.34	0.51
1:D:22:LEU:HD12	1:D:46:VAL:HG12	1.93	0.51
1:D:114:ILE:HG13	1:D:115:VAL:HG23	1.93	0.51
1:B:143:LYS:HA	1:B:225:ALA:HB1	1.93	0.51
1:C:211:LYS:HG2	1:C:213:TRP:CZ2	2.46	0.51
1:D:231:LEU:HD12	1:D:241:ILE:HD13	1.91	0.51
1:D:68:VAL:HG12	1:D:69:GLY:N	2.26	0.50
1:C:193:ASP:O	1:C:197:VAL:HG23	2.11	0.50
1:A:148:GLU:HG2	2:A:315:HOH:O	2.11	0.50
1:B:253:LEU:O	1:B:257:LYS:HG2	2.11	0.50
1:B:104:SER:OG	1:B:217:ALA:HB3	2.10	0.50
1:A:215:ILE:O	1:A:219:LEU:HG	2.11	0.50
1:D:43:VAL:HG11	1:D:95:ILE:CD1	2.41	0.50
1:A:158:GLY:HA3	1:A:207:GLU:OE2	2.12	0.49
1:C:69:GLY:HA2	1:C:213:TRP:CE3	2.47	0.49
1:C:207:GLU:CG	1:C:210:MSE:SE	3.09	0.49
1:D:43:VAL:HG11	1:D:95:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:PHE:CD1	1:D:212:PRO:HB2	2.48	0.49
1:D:210:MSE:HG2	1:D:215:ILE:HG23	1.94	0.49
1:A:153:ALA:HA	1:A:203:ASP:OD2	2.11	0.49
1:B:107:LEU:HB3	1:B:115:VAL:HB	1.94	0.49
1:C:20:GLN:HA	1:C:23:LYS:CD	2.42	0.49
1:C:107:LEU:HB3	1:C:115:VAL:HB	1.94	0.49
1:A:207:GLU:CG	1:A:210:MSE:SE	3.11	0.49
1:A:52:GLU:O	1:A:56:GLU:HB2	2.13	0.49
1:A:175:LYS:HD2	1:D:167:ILE:CD1	2.38	0.49
1:D:10:VAL:HG21	1:D:62:PHE:CE2	2.48	0.49
1:D:126:LEU:H	1:D:138:ASN:HD21	1.56	0.49
1:D:160:PRO:HG3	1:D:209:GLU:HG3	1.95	0.49
1:A:162:ARG:HH11	1:A:162:ARG:HG2	1.77	0.48
1:A:167:ILE:HD13	1:D:175:LYS:HG3	1.96	0.48
1:C:6:LYS:O	1:C:10:VAL:HG23	2.13	0.48
1:A:185:ARG:C	1:A:187:PRO:HD3	2.34	0.48
1:D:42:PHE:CG	1:D:43:VAL:N	2.79	0.48
1:D:157:TYR:CD1	1:D:184:MSE:HE2	2.49	0.48
1:D:257:LYS:HB3	1:D:262:VAL:CG1	2.43	0.48
1:B:169:ILE:O	1:B:173:ILE:HG13	2.14	0.48
1:C:165:ARG:NH2	1:C:240:ASP:OD2	2.44	0.48
1:A:211:LYS:HB2	1:A:214:ASP:OD2	2.14	0.47
1:D:123:PHE:O	1:D:125:LYS:HD2	2.13	0.47
1:D:192:VAL:HG12	1:D:196:MSE:HE2	1.96	0.47
1:A:185:ARG:NE	1:D:188:GLY:HA3	2.29	0.47
1:A:207:GLU:HG2	1:A:210:MSE:SE	2.64	0.47
1:D:164:ARG:HG2	1:D:164:ARG:HH11	1.79	0.47
1:D:257:LYS:HB3	1:D:262:VAL:HG12	1.96	0.47
1:A:185:ARG:HE	1:D:93:ASN:ND2	2.05	0.47
1:A:205:MSE:HG3	1:A:206:MSE:N	2.27	0.47
1:A:4:LEU:HD12	1:A:4:LEU:H	1.79	0.47
1:A:157:TYR:CZ	1:A:174:PHE:HE2	2.33	0.47
1:D:79:SER:O	1:D:80:GLU:HB3	2.13	0.47
1:D:165:ARG:NH1	1:D:240:ASP:OD1	2.48	0.47
1:D:210:MSE:HG2	1:D:215:ILE:CG2	2.45	0.47
1:B:254:GLN:HA	1:B:257:LYS:HE2	1.97	0.47
1:C:175:LYS:CG	1:C:176:ASP:N	2.77	0.47
1:B:28:LYS:HG3	2:B:339:HOH:O	2.15	0.47
1:C:155:VAL:O	1:C:184:MSE:HA	2.14	0.47
1:D:4:LEU:HA	1:D:7:TYR:HD2	1.80	0.47
1:B:137:VAL:HG13	1:B:137:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LYS:HE2	1:D:182:GLY:O	2.15	0.46
1:B:8:LEU:HD21	1:B:128:TRP:CE3	2.50	0.46
1:B:156:VAL:HA	1:B:185:ARG:O	2.15	0.46
1:B:205:MSE:HE2	1:B:241:ILE:CG2	2.45	0.46
1:B:192:VAL:HG12	1:B:196:MSE:HE2	1.97	0.46
1:C:180:GLU:HG3	1:C:251:PHE:CZ	2.51	0.46
1:A:80:GLU:O	1:A:109:LYS:HA	2.16	0.46
1:D:169:ILE:O	1:D:173:ILE:HG13	2.16	0.46
1:C:137:VAL:O	1:C:137:VAL:CG1	2.64	0.46
1:B:155:VAL:O	1:B:184:MSE:HA	2.15	0.46
1:B:182:GLY:O	1:C:92:LYS:HE2	2.15	0.46
1:C:165:ARG:NH2	1:C:240:ASP:CG	2.69	0.46
1:D:156:VAL:HG23	1:D:205:MSE:CB	2.46	0.46
1:A:8:LEU:HA	1:A:115:VAL:HG11	1.98	0.45
1:B:160:PRO:HG2	1:B:163:SER:OG	2.17	0.45
1:C:242:ILE:HD13	1:C:252:ILE:HG22	1.98	0.45
1:D:261:GLU:O	1:D:261:GLU:CG	2.38	0.45
1:D:42:PHE:CE1	1:D:44:SER:HB2	2.51	0.45
1:C:165:ARG:NH2	1:C:240:ASP:OD1	2.49	0.45
1:A:232:VAL:HB	1:A:240:ASP:HB2	1.99	0.45
1:C:205:MSE:HE1	1:C:207:GLU:HB2	1.96	0.45
1:A:155:VAL:O	1:A:184:MSE:HA	2.16	0.45
1:C:210:MSE:HE3	1:C:214:ASP:CB	2.46	0.45
1:C:8:LEU:HG	1:C:130:ALA:HB2	1.98	0.45
1:B:206:MSE:HA	1:B:241:ILE:O	2.17	0.45
1:C:175:LYS:HG3	1:C:176:ASP:N	2.31	0.45
1:D:167:ILE:HG13	1:D:168:SER:H	1.82	0.45
1:D:190:ALA:O	1:D:193:ASP:HB2	2.16	0.45
1:C:205:MSE:HE3	1:C:205:MSE:HB2	1.87	0.44
1:D:83:TRP:CE2	1:D:107:LEU:HD13	2.52	0.44
1:D:232:VAL:HG22	1:D:262:VAL:CG2	2.47	0.44
1:B:14:ALA:HB1	1:B:54:ILE:HG23	1.97	0.44
1:D:205:MSE:HE1	1:D:241:ILE:CG2	2.45	0.44
1:D:241:ILE:HD12	1:D:242:ILE:N	2.32	0.44
1:A:83:TRP:CE2	1:A:107:LEU:HD13	2.52	0.44
1:B:164:ARG:HD2	1:B:164:ARG:O	2.17	0.44
1:B:232:VAL:HG11	1:B:260:MSE:CE	2.48	0.44
1:C:53:ARG:NE	2:C:288:HOH:O	2.50	0.44
1:A:179:TYR:HE2	1:D:167:ILE:HD13	1.82	0.44
1:D:130:ALA:HB3	1:D:133:LEU:HD12	1.99	0.44
1:D:166:ASP:O	1:D:167:ILE:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:GLU:HA	1:C:113:PRO:HD3	1.86	0.44
1:A:186:ARG:HD2	1:D:157:TYR:OH	2.18	0.44
1:D:167:ILE:HG13	1:D:168:SER:N	2.33	0.44
1:B:8:LEU:HD21	1:B:128:TRP:CZ3	2.53	0.44
1:A:98:PHE:CD1	1:A:99:PRO:HD2	2.53	0.43
1:B:79:SER:O	1:B:80:GLU:HB2	2.18	0.43
1:B:92:LYS:CD	1:C:183:SER:HB3	2.46	0.43
1:C:3:ASN:O	1:C:4:LEU:C	2.56	0.43
1:D:175:LYS:HE2	1:D:175:LYS:HB3	1.80	0.43
1:A:3:ASN:HB2	1:A:7:TYR:CZ	2.53	0.43
1:A:6:LYS:HE3	1:A:62:PHE:CE1	2.52	0.43
1:A:114:ILE:O	1:A:130:ALA:HA	2.19	0.43
1:D:48:LYS:NZ	1:D:52:GLU:HG3	2.33	0.43
1:B:22:LEU:HD22	1:B:103:VAL:CG2	2.48	0.43
1:D:241:ILE:HD12	1:D:242:ILE:H	1.82	0.43
1:B:119:TYR:O	1:B:121:PRO:HD3	2.18	0.43
1:C:147:ASN:OD1	1:C:203:ASP:OD2	2.37	0.43
1:A:192:VAL:O	1:A:196:MSE:HG3	2.18	0.43
1:D:22:LEU:HD22	1:D:103:VAL:CG2	2.47	0.43
1:A:197:VAL:CG1	1:A:244:GLY:HA2	2.46	0.43
1:A:208:PHE:O	1:A:210:MSE:HE3	2.19	0.43
1:D:172:ASN:HB3	1:D:259:TYR:CE2	2.53	0.43
1:A:242:ILE:HG23	1:A:252:ILE:HG21	2.00	0.43
1:C:150:LEU:O	1:C:181:VAL:HA	2.18	0.43
1:A:211:LYS:HG2	2:A:293:HOH:O	2.19	0.42
1:C:177:VAL:O	1:C:181:VAL:HG22	2.20	0.42
1:B:6:LYS:HE3	1:B:62:PHE:HE1	1.84	0.42
1:B:229:TYR:HB2	1:B:241:ILE:HD11	2.01	0.42
1:A:6:LYS:HG2	1:A:62:PHE:HZ	1.84	0.42
1:A:203:ASP:HB3	1:A:248:LEU:HD23	2.02	0.42
1:C:93:ASN:HB3	1:C:98:PHE:HB3	2.01	0.42
1:D:150:LEU:O	1:D:181:VAL:HA	2.20	0.42
1:D:155:VAL:CG2	1:D:248:LEU:HD13	2.50	0.42
1:B:248:LEU:HD13	1:B:248:LEU:HA	1.88	0.42
1:C:212:PRO:HB3	1:C:236:PHE:HA	2.02	0.42
1:A:210:MSE:O	1:A:238:VAL:HA	2.19	0.41
1:C:207:GLU:HB3	1:C:241:ILE:CG2	2.50	0.41
1:D:177:VAL:CG2	1:D:252:ILE:HG22	2.48	0.41
1:D:203:ASP:HB3	1:D:245:ASN:HD21	1.85	0.41
1:C:153:ALA:CB	1:C:248:LEU:HD21	2.50	0.41
1:A:232:VAL:O	1:A:239:SER:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:PRO:HG3	1:D:209:GLU:CG	2.51	0.41
1:B:167:ILE:HD12	1:B:167:ILE:N	2.10	0.41
1:B:163:SER:HB3	1:B:209:GLU:OE2	2.21	0.41
1:B:205:MSE:CE	1:B:207:GLU:HG3	2.49	0.41
1:C:119:TYR:HB2	1:C:126:LEU:HD13	2.02	0.41
1:D:28:LYS:O	1:D:29:VAL:C	2.58	0.41
1:B:20:GLN:O	1:B:24:GLU:HG3	2.21	0.41
1:D:140:LYS:HE3	1:D:140:LYS:HB2	1.62	0.41
1:A:120:LEU:N	1:A:120:LEU:HD12	2.35	0.41
1:B:4:LEU:HA	1:B:7:TYR:CD2	2.55	0.41
1:D:205:MSE:CE	1:D:241:ILE:HG23	2.47	0.41
1:A:126:LEU:O	1:A:137:VAL:HA	2.21	0.41
1:A:137:VAL:O	1:A:137:VAL:CG1	2.67	0.41
1:A:210:MSE:HA	1:A:210:MSE:HE2	2.03	0.41
1:B:181:VAL:CG1	1:B:182:GLY:N	2.84	0.41
1:B:261:GLU:CD	1:B:261:GLU:N	2.72	0.41
1:C:43:VAL:O	1:C:43:VAL:HG13	2.21	0.41
1:C:164:ARG:NH1	2:C:316:HOH:O	2.48	0.41
1:D:8:LEU:O	1:D:12:LYS:HG3	2.21	0.41
1:D:51:GLU:HB2	1:D:87:PRO:CG	2.51	0.41
1:D:136:TYR:HA	1:D:140:LYS:O	2.21	0.41
1:D:248:LEU:HD23	1:D:248:LEU:HA	1.69	0.41
1:A:172:ASN:HD22	1:A:175:LYS:CE	2.33	0.40
1:A:161:SER:HA	1:D:178:PHE:CZ	2.54	0.40
1:A:61:PHE:CE1	1:C:56:GLU:HG3	2.55	0.40
1:A:79:SER:C	1:A:81:TYR:H	2.24	0.40
1:B:102:ALA:HB1	1:B:119:TYR:O	2.20	0.40
1:D:156:VAL:HG23	1:D:205:MSE:HB3	2.02	0.40
1:A:179:TYR:OH	1:D:167:ILE:HD13	2.22	0.40
1:C:131:LYS:NZ	1:C:223:LYS:NZ	2.69	0.40
1:B:50:SER:O	1:B:54:ILE:HG13	2.22	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	232/264 (88%)	223 (96%)	8 (3%)	1 (0%)	30	52
1	B	235/264 (89%)	221 (94%)	13 (6%)	1 (0%)	30	52
1	C	233/264 (88%)	221 (95%)	12 (5%)	0	100	100
1	D	232/264 (88%)	218 (94%)	12 (5%)	2 (1%)	14	31
All	All	932/1056 (88%)	883 (95%)	45 (5%)	4 (0%)	30	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	VAL
1	D	167	ILE
1	B	99	PRO
1	D	99	PRO

### 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	194/207 (94%)	188 (97%)	6 (3%)	35	62
1	B	197/207 (95%)	189 (96%)	8 (4%)	26	51
1	C	197/207 (95%)	190 (96%)	7 (4%)	30	56
1	D	196/207 (95%)	189 (96%)	7 (4%)	30	56
All	All	784/828 (95%)	756 (96%)	28 (4%)	30	56

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	148	GLU
1	A	150	LEU
1	A	162	ARG

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Mol	Chain	Res	Type
1	A	194	LEU
1	A	261	GLU
1	B	23	LYS
1	B	45	TYR
1	B	59	LEU
1	B	126	LEU
1	B	146	ASP
1	B	167	ILE
1	B	234	GLU
1	B	261	GLU
1	C	8	LEU
1	C	45	TYR
1	C	64	ASP
1	C	70	GLU
1	C	79	SER
1	C	88	LEU
1	C	147	ASN
1	D	6	LYS
1	D	150	LEU
1	D	166	ASP
1	D	210	MSE
1	D	231	LEU
1	D	253	LEU
1	D	262	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	HIS
1	A	172	ASN
1	C	96	ASN
1	D	93	ASN
1	D	96	ASN
1	D	138	ASN
1	D	147	ASN

### 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 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	232/264 (87%)	-0.43	6 (2%) 57 51	12, 26, 62, 95	0
1	B	234/264 (88%)	-0.25	8 (3%) 48 42	12, 31, 71, 93	0
1	C	234/264 (88%)	-0.36	7 (2%) 52 46	12, 28, 62, 93	0
1	D	234/264 (88%)	-0.31	13 (5%) 31 25	11, 28, 78, 101	0
All	All	934/1056 (88%)	-0.34	34 (3%) 46 40	11, 28, 70, 101	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	43	VAL	5.6
1	D	29	VAL	4.4
1	D	161	SER	4.1
1	A	263	ALA	4.0
1	B	79	SER	4.0
1	C	29	VAL	3.8
1	D	42	PHE	3.6
1	D	43	VAL	3.6
1	A	44	SER	3.5
1	C	263	ALA	3.3
1	D	263	ALA	3.3
1	D	148	GLU	3.2
1	D	69	GLY	3.2
1	A	261	GLU	2.9
1	C	79	SER	2.7
1	D	147	ASN	2.7
1	B	263	ALA	2.7
1	C	161	SER	2.6
1	B	80	GLU	2.6
1	D	167	ILE	2.6
1	D	252	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	44	SER	2.5
1	D	163	SER	2.4
1	B	44	SER	2.4
1	D	79	SER	2.3
1	B	161	SER	2.3
1	A	3	ASN	2.1
1	C	252	ILE	2.1
1	D	80	GLU	2.1
1	B	29	VAL	2.1
1	B	256	ALA	2.1
1	A	4	LEU	2.0
1	A	45	TYR	2.0
1	B	163	SER	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.