



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 11:00 PM EDT

PDB ID : 2Z04  
Title : Crystal structure of phosphoribosylaminoimidazole carboxylase ATPase subunit from Aquifex aeolicus  
Authors : Okada, K.; Tamura, S.; Baba, S.; Kanagawa, M.; Kawai, G.; Sampei, G.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2007-05-06  
Resolution : 2.35 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	:	2.37.1
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)	:	2.37.1

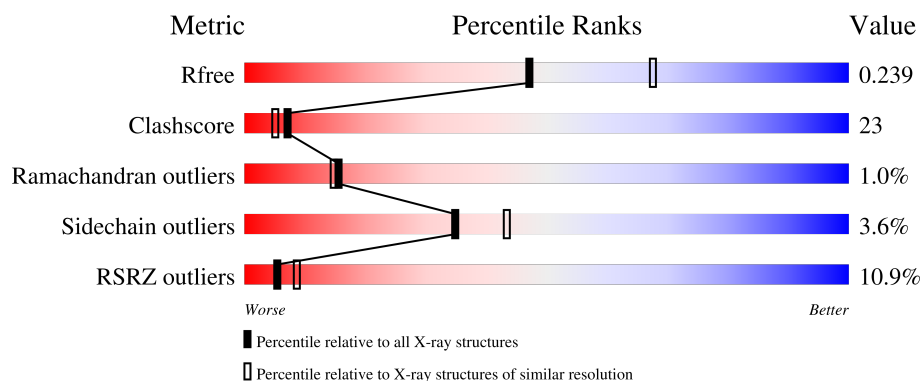
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	365	<div> <div>9%</div> <div>52%</div> <div>31%</div> <div>15%</div> </div>
1	B	365	<div> <div>10%</div> <div>52%</div> <div>33%</div> <div>11%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5205 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 Phosphoribosylaminoimidazole carboxylase ATPase subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	Se	0	0	0
			2509	1633	417	450	5	4			
1	B	325	Total	C	N	O	S	Se	0	0	0
			2646	1719	440	478	5	4			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

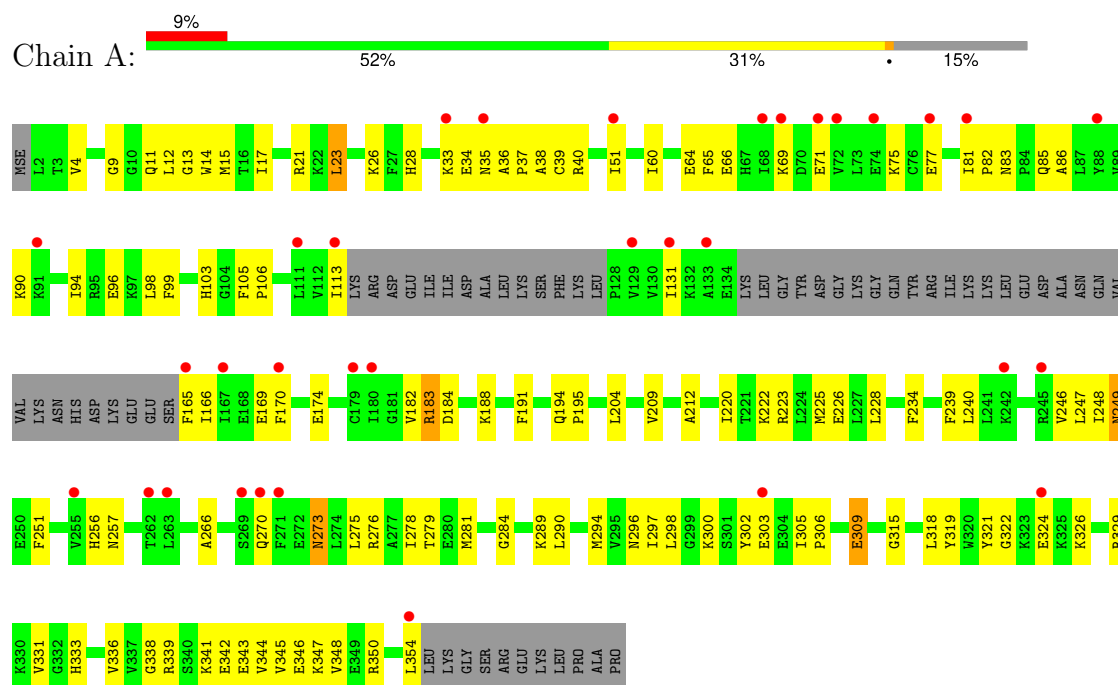
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total 17	O 17	0	0
3	B	23	Total 23	O 23	0	0

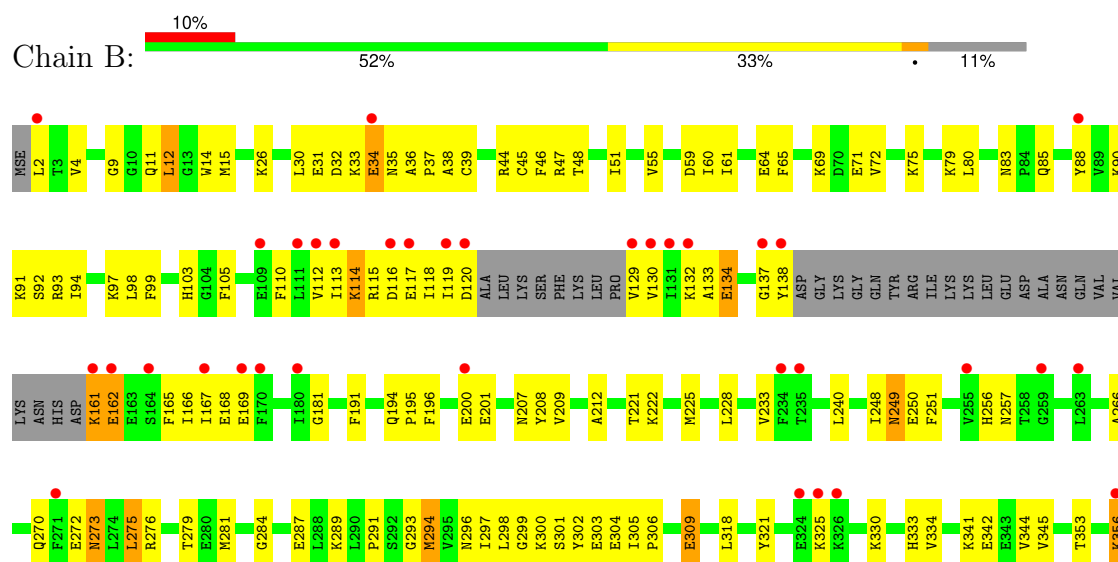
### 3 Residue-property plots

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: Phosphoribosylaminoimidazole carboxylase ATPase subunit



#### • Molecule 1: Phosphoribosylaminoimidazole carboxylase ATPase subunit



GLY
SER
ARG
GLU
LYS
LEU
PRO
ALA
PRO

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.29Å 55.05Å 74.54Å 93.93° 101.54° 114.23°	Depositor
Resolution (Å)	32.41 – 2.35 32.41 – 2.35	Depositor EDS
% Data completeness (in resolution range)	94.0 (32.41-2.35) 98.4 (32.41-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.85 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.232 , 0.267 0.233 , 0.239	Depositor DCC
$R_{free}$ test set	1492 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.4	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 62.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.03% 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

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0/2559	0.59	0/3438
1	B	0.37	0/2696	0.59	0/3618
All	All	0.36	0/5255	0.59	0/7056

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	2509	0	2564	111	0
1	B	2646	0	2708	126	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	17	0	0	0	0
3	B	23	0	0	0	0
All	All	5205	0	5272	236	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 23.

All (236) 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:273:ASN:HD21	1:A:284:GLY:H	1.06	1.00
1:B:115:ARG:HE	1:B:162:GLU:H	1.17	0.93
1:B:129:VAL:HG22	1:B:169:GLU:HG2	1.55	0.85
1:A:321:TYR:OH	1:A:333:HIS:HD2	1.62	0.82
1:B:276:ARG:HA	1:B:281:MSE:HE3	1.59	0.82
1:B:341:LYS:O	1:B:345:VAL:HG23	1.80	0.80
1:B:93:ARG:HD2	1:B:132:LYS:HD3	1.64	0.79
1:A:81:ILE:HB	1:A:82:PRO:HD3	1.67	0.77
1:A:306:PRO:HB2	1:A:309:GLU:CG	2.15	0.77
1:A:184:ASP:OD2	1:A:188:LYS:HB3	1.86	0.76
1:B:257:ASN:HD22	1:B:330:LYS:NZ	1.84	0.76
1:A:273:ASN:ND2	1:A:284:GLY:H	1.82	0.75
1:B:195:PRO:HB3	1:B:209:VAL:HG13	1.69	0.75
1:A:257:ASN:HD21	1:A:296:ASN:HD21	1.35	0.75
1:B:273:ASN:HD21	1:B:284:GLY:H	1.33	0.74
1:B:115:ARG:HE	1:B:162:GLU:N	1.85	0.74
1:B:98:LEU:HD21	1:B:112:VAL:HG21	1.67	0.74
1:B:302:TYR:O	1:B:305:ILE:HG12	1.89	0.73
1:B:306:PRO:HB2	1:B:309:GLU:CG	2.20	0.72
1:A:324:GLU:HB3	1:A:329:ARG:HH12	1.57	0.70
1:B:115:ARG:NE	1:B:162:GLU:H	1.86	0.70
1:B:318:LEU:HD23	1:B:334:VAL:HG22	1.73	0.70
1:A:306:PRO:O	1:A:309:GLU:HG2	1.91	0.69
1:A:183:ARG:NH1	1:A:226:GLU:HA	2.08	0.68
1:B:113:ILE:HG13	1:B:117:GLU:HB2	1.74	0.68
1:A:81:ILE:HG21	1:A:278:ILE:HB	1.77	0.67
1:B:298:LEU:O	1:B:300:LYS:HG3	1.93	0.67
1:B:301:SER:HB3	1:B:325:LYS:HD2	1.77	0.67
1:B:4:VAL:HG22	1:B:60:ILE:HD11	1.76	0.67
1:B:321:TYR:OH	1:B:333:HIS:HD2	1.78	0.67
1:A:94:ILE:HA	1:A:166:ILE:HD11	1.77	0.66
1:B:61:ILE:O	1:B:80:LEU:HD12	1.95	0.66
1:B:11:GLN:O	1:B:15:MSE:HG3	1.96	0.65
1:A:40:ARG:HH22	1:A:322:GLY:HA3	1.62	0.65
1:B:306:PRO:HB2	1:B:309:GLU:HG2	1.78	0.65
1:A:81:ILE:HG21	1:A:278:ILE:CB	2.26	0.64
1:A:276:ARG:HA	1:A:281:MSE:HE3	1.79	0.64
1:B:256:HIS:H	1:B:270:GLN:HE22	1.46	0.64
1:B:257:ASN:HD22	1:B:330:LYS:HZ2	1.47	0.63
1:A:343:GLU:HG2	1:A:347:LYS:HE3	1.79	0.63
1:B:94:ILE:HG12	1:B:166:ILE:CG1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:THR:O	1:B:225:MSE:HG3	1.98	0.63
1:B:279:THR:OG1	1:B:281:MSE:HE2	2.00	0.62
1:A:105:PHE:HB3	1:A:248:ILE:HD12	1.81	0.62
1:A:306:PRO:HB2	1:A:309:GLU:HG2	1.80	0.62
1:A:302:TYR:O	1:A:305:ILE:HG12	2.00	0.61
1:B:30:LEU:HD11	1:B:48:THR:HA	1.82	0.61
1:A:83:ASN:HD21	1:A:85:GLN:HB2	1.64	0.61
1:B:303:GLU:H	1:B:303:GLU:CD	2.04	0.61
1:B:90:LYS:HD2	1:B:251:PHE:O	2.01	0.61
1:B:99:PHE:O	1:B:103:HIS:HD2	1.83	0.60
1:A:279:THR:OG1	1:A:281:MSE:HE2	2.02	0.59
1:A:321:TYR:OH	1:A:333:HIS:CD2	2.51	0.59
1:A:83:ASN:ND2	1:A:85:GLN:H	2.00	0.59
1:B:83:ASN:ND2	1:B:85:GLN:HG3	2.18	0.59
1:B:113:ILE:HD11	1:B:117:GLU:HB3	1.84	0.59
1:A:194:GLN:HB2	1:A:212:ALA:O	2.01	0.59
1:A:204:LEU:HD12	1:A:296:ASN:ND2	2.18	0.59
1:A:256:HIS:H	1:A:270:GLN:HE22	1.51	0.59
1:A:324:GLU:HB3	1:A:329:ARG:NH1	2.17	0.59
1:B:273:ASN:HD21	1:B:284:GLY:N	2.00	0.59
1:B:353:THR:HG23	1:B:356:LYS:HE2	1.84	0.58
1:A:303:GLU:CD	1:A:303:GLU:H	2.07	0.58
1:B:273:ASN:ND2	1:B:284:GLY:H	2.00	0.57
1:A:86:ALA:HB2	1:A:228:LEU:HD13	1.86	0.57
1:B:294:MSE:HE1	1:B:296:ASN:OD1	2.03	0.57
1:A:81:ILE:HG13	1:A:278:ILE:HB	1.86	0.57
1:A:105:PHE:HZ	1:A:223:ARG:HG3	1.68	0.57
1:B:294:MSE:HE1	1:B:296:ASN:CG	2.25	0.57
1:B:61:ILE:O	1:B:80:LEU:HA	2.05	0.56
1:A:15:MSE:HE1	1:A:333:HIS:NE2	2.21	0.56
1:B:309:GLU:CD	1:B:309:GLU:H	2.08	0.56
1:A:318:LEU:HD13	1:A:318:LEU:C	2.25	0.56
1:B:300:LYS:NZ	1:B:300:LYS:HB3	2.20	0.56
1:A:83:ASN:ND2	1:A:85:GLN:HG3	2.22	0.55
1:A:306:PRO:HB2	1:A:309:GLU:HG3	1.87	0.55
1:B:249:ASN:HD22	1:B:249:ASN:C	2.09	0.55
1:B:306:PRO:O	1:B:309:GLU:HG2	2.06	0.55
1:B:44:ARG:HH11	1:B:46:PHE:HZ	1.55	0.55
1:B:257:ASN:ND2	1:B:330:LYS:NZ	2.54	0.55
1:A:273:ASN:HD21	1:A:284:GLY:N	1.89	0.55
1:B:272:GLU:O	1:B:276:ARG:HG3	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LYS:NZ	1:A:300:LYS:HB3	2.22	0.54
1:B:194:GLN:HB2	1:B:212:ALA:O	2.07	0.54
1:B:9:GLY:O	1:B:36:ALA:HB1	2.07	0.54
1:B:129:VAL:CG2	1:B:169:GLU:HG2	2.34	0.54
1:A:105:PHE:CZ	1:A:223:ARG:HG3	2.43	0.54
1:A:341:LYS:O	1:A:345:VAL:HG23	2.08	0.54
1:A:36:ALA:HB3	1:A:39:CYS:SG	2.48	0.53
1:A:257:ASN:HD21	1:A:296:ASN:ND2	2.04	0.53
1:B:161:LYS:O	1:B:161:LYS:HG2	2.08	0.53
1:A:4:VAL:HG22	1:A:60:ILE:HD11	1.89	0.53
1:A:9:GLY:HA2	1:A:38:ALA:HB3	1.89	0.53
1:B:88:TYR:HD1	1:B:91:LYS:HZ1	1.56	0.53
1:B:321:TYR:OH	1:B:333:HIS:CD2	2.61	0.53
1:B:191:PHE:HZ	1:B:222:LYS:HB2	1.74	0.53
1:B:115:ARG:HE	1:B:161:LYS:HA	1.74	0.52
1:A:83:ASN:HD21	1:A:85:GLN:CB	2.22	0.52
1:B:99:PHE:O	1:B:103:HIS:CD2	2.63	0.52
1:A:113:ILE:O	1:A:165:PHE:HB2	2.10	0.52
1:A:297:ILE:HG22	1:A:331:VAL:CG2	2.40	0.52
1:A:294:MSE:HE1	1:A:296:ASN:OD1	2.10	0.51
1:A:249:ASN:C	1:A:249:ASN:HD22	2.13	0.51
1:A:222:LYS:O	1:A:226:GLU:HG3	2.09	0.51
1:B:34:GLU:CD	1:B:34:GLU:H	2.14	0.51
1:B:93:ARG:CD	1:B:132:LYS:HD3	2.39	0.51
1:B:115:ARG:NE	1:B:161:LYS:HA	2.25	0.51
1:B:118:ILE:O	1:B:120:ASP:N	2.43	0.51
1:B:138:TYR:HE1	1:B:161:LYS:HD2	1.75	0.51
1:A:64:GLU:HG2	1:A:65:PHE:CD2	2.45	0.51
1:B:129:VAL:HG22	1:B:169:GLU:CG	2.36	0.51
1:B:110:PHE:HA	1:B:167:ILE:O	2.11	0.51
1:B:12:LEU:HD22	1:B:65:PHE:CZ	2.45	0.51
1:B:301:SER:OG	1:B:304:GLU:HG3	2.11	0.51
1:A:204:LEU:HD12	1:A:296:ASN:HD21	1.77	0.50
1:B:300:LYS:HZ1	1:B:304:GLU:C	2.15	0.50
1:B:9:GLY:HA2	1:B:38:ALA:HB3	1.93	0.50
1:B:15:MSE:HE1	1:B:333:HIS:NE2	2.27	0.49
1:A:81:ILE:HG21	1:A:278:ILE:CG2	2.42	0.49
1:B:249:ASN:C	1:B:249:ASN:ND2	2.65	0.49
1:A:51:ILE:HD13	1:A:75:LYS:HD2	1.94	0.49
1:B:94:ILE:HG12	1:B:166:ILE:HG13	1.94	0.49
1:B:297:ILE:CD1	1:B:318:LEU:HD21	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LYS:N	1:B:161:LYS:HD3	2.28	0.49
1:A:298:LEU:O	1:A:300:LYS:HG3	2.13	0.48
1:A:26:LYS:HE2	1:A:28:HIS:NE2	2.28	0.48
1:A:297:ILE:HG22	1:A:331:VAL:HG23	1.94	0.48
1:A:290:LEU:HD12	1:A:338:GLY:O	2.13	0.48
1:B:31:GLU:OE1	1:B:33:LYS:HB2	2.13	0.48
1:A:34:GLU:HG3	1:A:35:ASN:H	1.78	0.48
1:A:83:ASN:HD21	1:A:85:GLN:CG	2.27	0.48
1:A:131:ILE:HA	1:A:166:ILE:O	2.14	0.48
1:A:81:ILE:HG21	1:A:278:ILE:HG22	1.94	0.48
1:B:39:CYS:SG	1:B:45:CYS:SG	3.12	0.48
1:B:69:LYS:HE2	1:B:71:GLU:OE1	2.14	0.48
1:B:291:PRO:C	1:B:344:VAL:HG21	2.34	0.48
1:B:55:VAL:HG21	1:B:75:LYS:O	2.14	0.47
1:A:169:GLU:HG2	1:A:170:PHE:N	2.30	0.47
1:B:115:ARG:NH1	1:B:116:ASP:OD2	2.48	0.47
1:A:69:LYS:HE2	1:A:71:GLU:OE1	2.14	0.47
1:A:326:LYS:HB2	1:A:329:ARG:HD2	1.95	0.47
1:B:303:GLU:CD	1:B:303:GLU:N	2.67	0.47
1:A:315:GLY:O	1:A:336:VAL:HA	2.14	0.47
1:B:114:LYS:O	1:B:118:ILE:HG13	2.15	0.47
1:A:34:GLU:HG3	1:A:35:ASN:N	2.29	0.47
1:B:168:GLU:O	1:B:168:GLU:HG3	2.14	0.47
1:A:309:GLU:HB2	1:A:354:LEU:HD13	1.97	0.47
1:A:13:GLY:O	1:A:17:ILE:HG13	2.15	0.46
1:A:182:VAL:HG11	1:A:273:ASN:HB3	1.98	0.46
1:A:344:VAL:O	1:A:348:VAL:HG23	2.15	0.46
1:B:300:LYS:HB3	1:B:300:LYS:HZ3	1.80	0.46
1:A:220:ILE:CG2	1:A:248:ILE:HD11	2.46	0.46
1:B:113:ILE:HG13	1:B:117:GLU:CB	2.42	0.46
1:B:273:ASN:HD22	1:B:273:ASN:HA	1.54	0.46
1:B:55:VAL:O	1:B:79:LYS:NZ	2.40	0.46
1:B:2:LEU:HD12	1:B:59:ASP:OD1	2.16	0.46
1:B:256:HIS:H	1:B:270:GLN:NE2	2.12	0.46
1:A:37:PRO:O	1:A:40:ARG:HB3	2.16	0.46
1:A:222:LYS:HA	1:A:225:MSE:HE3	1.98	0.46
1:B:51:ILE:CD1	1:B:72:VAL:HG13	2.46	0.46
1:A:12:LEU:HB2	1:A:64:GLU:HG3	1.97	0.45
1:A:81:ILE:HB	1:A:82:PRO:CD	2.43	0.45
1:A:94:ILE:HG12	1:A:166:ILE:HD11	1.98	0.45
1:A:96:GLU:O	1:A:99:PHE:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ILE:HD11	1:B:165:PHE:CD2	2.51	0.45
1:B:138:TYR:CE1	1:B:161:LYS:HD2	2.50	0.45
1:B:129:VAL:HG13	1:B:169:GLU:HG2	1.98	0.45
1:A:195:PRO:HB3	1:A:209:VAL:HG13	1.99	0.45
1:A:83:ASN:ND2	1:A:85:GLN:CG	2.80	0.44
1:B:94:ILE:N	1:B:166:ILE:HD11	2.32	0.44
1:B:93:ARG:O	1:B:97:LYS:HD3	2.18	0.44
1:A:90:LYS:HD2	1:A:251:PHE:O	2.16	0.44
1:A:17:ILE:O	1:A:21:ARG:HG2	2.17	0.44
1:B:208:TYR:HA	1:B:293:GLY:HA2	1.99	0.44
1:A:294:MSE:HE3	1:A:333:HIS:HB2	1.99	0.44
1:A:106:PRO:O	1:A:247:LEU:HA	2.18	0.44
1:B:342:GLU:H	1:B:342:GLU:CD	2.20	0.44
1:B:83:ASN:HD22	1:B:85:GLN:HG3	1.81	0.43
1:B:266:ALA:O	1:B:289:LYS:HE3	2.18	0.43
1:A:346:GLU:O	1:A:350:ARG:HG3	2.18	0.43
1:B:32:ASP:HA	1:B:47:ARG:CD	2.48	0.43
1:A:339:ARG:HH12	1:B:287:GLU:HG2	1.83	0.43
1:B:92:SER:OG	1:B:134:GLU:HG2	2.19	0.43
1:B:196:PHE:O	1:B:207:ASN:HB2	2.18	0.43
1:A:174:GLU:N	1:A:240:LEU:O	2.49	0.43
1:B:138:TYR:CD1	1:B:138:TYR:N	2.83	0.43
1:B:9:GLY:O	1:B:37:PRO:HD2	2.19	0.43
1:B:200:GLU:O	1:B:201:GLU:HB2	2.19	0.43
1:B:353:THR:O	1:B:356:LYS:HG3	2.18	0.43
1:A:228:LEU:HD12	1:A:234:PHE:CE2	2.54	0.42
1:B:32:ASP:O	1:B:47:ARG:NH1	2.50	0.42
1:B:133:ALA:HB2	1:B:165:PHE:CE1	2.54	0.42
1:B:341:LYS:O	1:B:341:LYS:HD2	2.19	0.42
1:A:11:GLN:O	1:A:14:TRP:HB3	2.19	0.42
1:A:183:ARG:NH1	1:A:225:MSE:O	2.50	0.42
1:A:184:ASP:OD2	1:A:188:LYS:HE2	2.18	0.42
1:B:71:GLU:H	1:B:71:GLU:CD	2.22	0.42
1:B:306:PRO:HB2	1:B:309:GLU:HG3	1.99	0.42
1:A:257:ASN:ND2	1:A:296:ASN:HD21	2.09	0.42
1:B:83:ASN:ND2	1:B:85:GLN:CG	2.83	0.42
1:B:14:TRP:CE3	1:B:15:MSE:HG2	2.54	0.42
1:B:257:ASN:ND2	1:B:330:LYS:HZ3	2.18	0.42
1:B:341:LYS:HD2	1:B:341:LYS:C	2.40	0.42
1:A:12:LEU:HD22	1:A:65:PHE:CZ	2.54	0.42
1:A:239:PHE:O	1:A:246:VAL:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:PHE:HB3	1:B:248:ILE:HD12	2.01	0.42
1:A:220:ILE:HG21	1:A:248:ILE:HD11	2.01	0.42
1:B:275:LEU:HD12	1:B:275:LEU:HA	1.84	0.42
1:A:191:PHE:HZ	1:A:222:LYS:HB2	1.84	0.41
1:B:26:LYS:HB3	1:B:26:LYS:HE2	1.84	0.41
1:B:114:LYS:HD2	1:B:114:LYS:N	2.35	0.41
1:A:318:LEU:HD22	1:A:319:TYR:N	2.34	0.41
1:B:257:ASN:ND2	1:B:330:LYS:HD3	2.34	0.41
1:B:85:GLN:NE2	1:B:228:LEU:HA	2.34	0.41
1:A:99:PHE:O	1:A:103:HIS:HD2	2.03	0.41
1:B:250:GLU:HG2	1:B:251:PHE:N	2.36	0.41
1:A:94:ILE:CA	1:A:166:ILE:HD11	2.47	0.41
1:A:183:ARG:HG2	1:A:188:LYS:O	2.21	0.41
1:B:181:GLY:O	1:B:233:VAL:HA	2.21	0.41
1:A:71:GLU:H	1:A:71:GLU:CD	2.24	0.41
1:A:183:ARG:HH12	1:A:226:GLU:HA	1.84	0.41
1:A:249:ASN:C	1:A:249:ASN:ND2	2.74	0.41
1:A:266:ALA:O	1:A:289:LYS:HE3	2.20	0.41
1:A:342:GLU:OE2	1:A:342:GLU:N	2.50	0.41
1:B:51:ILE:HD12	1:B:72:VAL:HG13	2.03	0.41
1:A:33:LYS:HE2	1:A:33:LYS:HB3	1.90	0.40
1:A:273:ASN:HD22	1:A:273:ASN:HA	1.67	0.40
1:A:26:LYS:CE	1:A:28:HIS:NE2	2.84	0.40
1:B:64:GLU:HG2	1:B:65:PHE:CD2	2.56	0.40
1:B:297:ILE:HD11	1:B:318:LEU:CD2	2.51	0.40
1:A:321:TYR:N	1:A:321:TYR:CD2	2.90	0.40
1:B:39:CYS:HB3	1:B:45:CYS:SG	2.62	0.40
1:B:129:VAL:HG12	1:B:130:VAL:N	2.37	0.40
1:A:23:LEU:HD12	1:A:23:LEU:HA	1.93	0.40
1:A:228:LEU:HD12	1:A:234:PHE:HE2	1.87	0.40
1:A:183:ARG:HH11	1:A:225:MSE:C	2.23	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	303/365 (83%)	289 (95%)	13 (4%)	1 (0%)	41	47
1	B	319/365 (87%)	302 (95%)	12 (4%)	5 (2%)	9	8
All	All	622/730 (85%)	591 (95%)	25 (4%)	6 (1%)	15	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	119	ILE
1	A	77	GLU
1	B	134	GLU
1	B	35	ASN
1	B	137	GLY
1	B	299	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/318 (86%)	266 (97%)	8 (3%)	42	52
1	B	289/318 (91%)	277 (96%)	12 (4%)	30	36
All	All	563/636 (88%)	543 (96%)	20 (4%)	35	43

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	66	GLU
1	A	98	LEU
1	A	183	ARG
1	A	249	ASN
1	A	273	ASN
1	A	275	LEU

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Mol	Chain	Res	Type
1	A	309	GLU
1	B	12	LEU
1	B	34	GLU
1	B	114	LYS
1	B	161	LYS
1	B	162	GLU
1	B	240	LEU
1	B	249	ASN
1	B	273	ASN
1	B	275	LEU
1	B	294	MSE
1	B	309	GLU
1	B	356	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	83	ASN
1	A	85	GLN
1	A	103	HIS
1	A	249	ASN
1	A	257	ASN
1	A	260	HIS
1	A	270	GLN
1	A	273	ASN
1	A	333	HIS
1	B	50	GLN
1	B	83	ASN
1	B	85	GLN
1	B	103	HIS
1	B	249	ASN
1	B	257	ASN
1	B	270	GLN
1	B	273	ASN
1	B	333	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	B	357	-	4,4,4	0.44	0	6,6,6	0.14	0
2	SO4	A	1	-	4,4,4	0.58	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	305/365 (83%)	0.76	33 (10%) 5 9	22, 51, 79, 111	0
1	B	321/365 (87%)	0.73	35 (10%) 5 9	22, 48, 88, 133	0
All	All	626/730 (85%)	0.74	68 (10%) 5 9	22, 49, 85, 133	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	ILE	8.2
1	A	165	PHE	7.0
1	B	137	GLY	6.0
1	B	138	TYR	5.8
1	B	131	ILE	5.6
1	B	112	VAL	5.4
1	A	88	TYR	5.0
1	A	170	PHE	4.7
1	A	113	ILE	4.6
1	A	131	ILE	4.6
1	B	113	ILE	4.4
1	B	129	VAL	4.3
1	B	356	LYS	4.1
1	A	133	ALA	4.0
1	B	162	GLU	3.9
1	A	167	ILE	3.9
1	B	119	ILE	3.7
1	A	263	LEU	3.7
1	A	111	LEU	3.6
1	B	116	ASP	3.5
1	B	164	SER	3.4
1	B	263	LEU	3.4
1	B	271	PHE	3.4
1	B	111	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	324	GLU	3.3
1	A	51	ILE	3.3
1	B	167	ILE	3.3
1	B	170	PHE	3.2
1	A	242	LYS	3.2
1	B	130	VAL	3.2
1	B	180	ILE	3.1
1	B	169	GLU	3.1
1	B	88	TYR	3.1
1	A	68	ILE	3.0
1	B	117	GLU	3.0
1	A	180	ILE	2.8
1	A	255	VAL	2.8
1	A	324	GLU	2.8
1	A	262	THR	2.8
1	B	34	GLU	2.6
1	A	35	ASN	2.6
1	B	255	VAL	2.5
1	A	129	VAL	2.4
1	A	245	ARG	2.4
1	B	120	ASP	2.4
1	B	132	LYS	2.4
1	A	269	SER	2.3
1	B	2	LEU	2.3
1	A	354	LEU	2.3
1	A	71	GLU	2.2
1	A	72	VAL	2.2
1	B	259	GLY	2.2
1	A	271	PHE	2.2
1	B	234	PHE	2.2
1	B	161	LYS	2.2
1	A	303	GLU	2.2
1	A	33	LYS	2.1
1	A	69	LYS	2.1
1	B	325	LYS	2.1
1	A	74	GLU	2.1
1	B	326	LYS	2.1
1	B	200	GLU	2.1
1	B	235	THR	2.1
1	A	91	LYS	2.1
1	A	270	GLN	2.0
1	B	109	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	179	CYS	2.0
1	A	77	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	SO4	B	357	5/5	0.94	0.14	71,71,73,73	0
2	SO4	A	1	5/5	0.95	0.12	69,70,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.