



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 07:50 pm BST

PDB ID : 2P4W
Title : Crystal structure of heat shock regulator from *Pyrococcus furiosus*
Authors : Liu, W.; Vierke, G.; Panjikar, S.; Thomm, M.; Ladenstein, R.
Deposited on : 2007-03-13
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.11
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) : 2.11

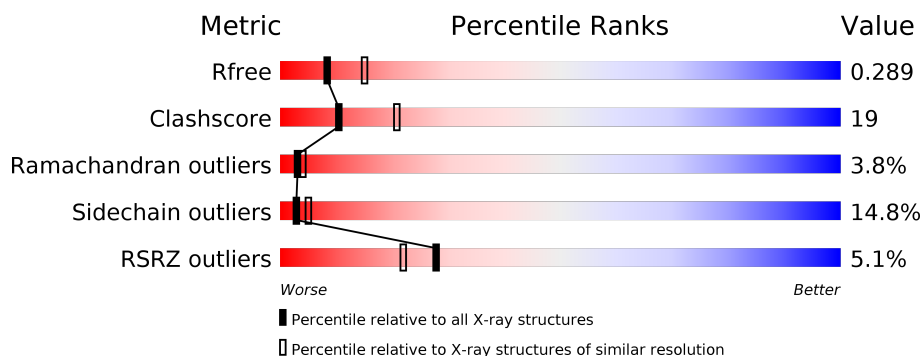
1 Overall quality at a glance

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	202	<div> <div>4%</div> <div> <div></div> <div>52%</div> <div>34%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	202	<div> <div>6%</div> <div> <div></div> <div>64%</div> <div>24%</div> <div>8%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3360 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 Transcriptional regulatory protein arsR family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	19	0	0
			1650	1049	295	301	5			
1	B	198	Total	C	N	O	S	0	0	0
			1658	1055	296	302	5			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		

Continued on next page...

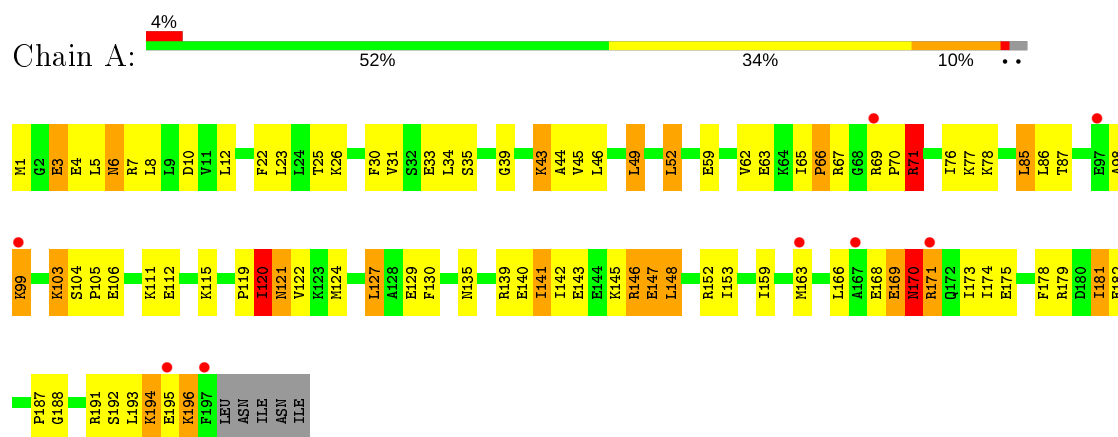
Continued from previous page...

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

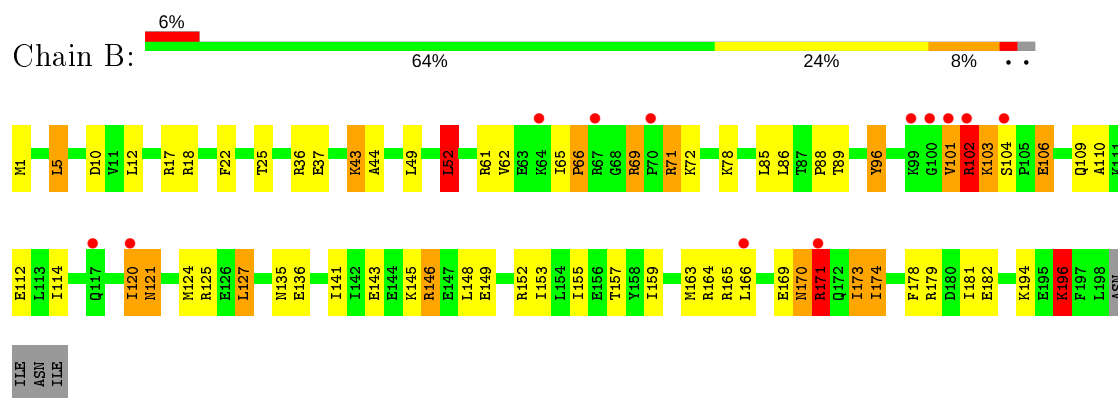
3 Residue-property plots [i](#)

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: Transcriptional regulatory protein arsR family



- Molecule 1: Transcriptional regulatory protein arsR family



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	52.39 Å 82.85 Å 114.49 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.66 – 2.60 38.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.66-2.60) 98.8 (38.65-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.54 (at 2.61 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.252 , 0.305 0.241 , 0.289	Depositor DCC
R_{free} test set	786 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3360	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7817e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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	1.28	15/1672 (0.9%)	1.06	7/2236 (0.3%)
1	B	1.44	15/1680 (0.9%)	1.29	9/2247 (0.4%)
All	All	1.36	30/3352 (0.9%)	1.18	16/4483 (0.4%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	ARG	CZ-NH1	25.88	1.66	1.33
1	A	170	ASN	CG-OD1	19.00	1.65	1.24
1	B	171	ARG	CZ-NH2	17.36	1.55	1.33
1	B	171	ARG	CD-NE	13.04	1.68	1.46
1	B	102	ARG	NE-CZ	12.52	1.49	1.33
1	B	102	ARG	CZ-NH1	12.30	1.49	1.33
1	A	67	ARG	CZ-NH1	11.12	1.47	1.33
1	A	67	ARG	CZ-NH2	9.77	1.45	1.33
1	A	62	VAL	CB-CG2	9.77	1.73	1.52
1	B	171	ARG	NE-CZ	9.61	1.45	1.33
1	A	67	ARG	NE-CZ	9.23	1.45	1.33
1	A	120	ILE	CA-CB	-8.71	1.34	1.54
1	A	63	GLU	CA-CB	-7.97	1.36	1.53
1	A	62	VAL	CB-CG1	7.97	1.69	1.52
1	A	169	GLU	CB-CG	-7.93	1.37	1.52
1	B	96	TYR	CE1-CZ	7.79	1.48	1.38
1	B	96	TYR	CG-CD2	7.01	1.48	1.39
1	A	67	ARG	CG-CD	6.77	1.68	1.51
1	B	102	ARG	CZ-NH2	6.28	1.41	1.33
1	A	140	GLU	CG-CD	5.97	1.60	1.51
1	A	67	ARG	CD-NE	5.93	1.56	1.46
1	A	147	GLU	CG-CD	5.64	1.60	1.51
1	A	146	ARG	CB-CG	-5.62	1.37	1.52
1	B	96	TYR	CG-CD1	5.58	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	96	TYR	CE2-CZ	5.56	1.45	1.38
1	B	37	GLU	CG-CD	5.47	1.60	1.51
1	A	3	GLU	CB-CG	5.32	1.62	1.52
1	B	102	ARG	CG-CD	5.31	1.65	1.51
1	B	136	GLU	CG-CD	5.18	1.59	1.51
1	B	102	ARG	CD-NE	5.02	1.54	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	ARG	NE-CZ-NH2	-29.94	105.33	120.30
1	B	102	ARG	NE-CZ-NH2	-12.88	113.86	120.30
1	B	171	ARG	NE-CZ-NH1	11.49	126.05	120.30
1	B	171	ARG	CD-NE-CZ	-10.86	108.39	123.60
1	A	62	VAL	CG1-CB-CG2	-10.78	93.65	110.90
1	B	146	ARG	NE-CZ-NH2	-10.35	115.13	120.30
1	B	102	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	B	171	ARG	NH1-CZ-NH2	7.98	128.18	119.40
1	B	146	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	A	120	ILE	CB-CA-C	7.27	126.13	111.60
1	B	52	LEU	CA-CB-CG	6.98	131.36	115.30
1	A	170	ASN	OD1-CG-ND2	6.76	137.45	121.90
1	A	67	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	52	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	169	GLU	CA-CB-CG	5.32	125.11	113.40
1	A	85	LEU	CA-CB-CG	5.08	126.98	115.30

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	1650	0	1730	80	0
1	B	1658	0	1741	68	0
2	A	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	24	0	0	3	0
3	B	23	0	0	1	0
All	All	3360	0	3471	125	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 19.

All (125) 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:171:ARG:CD	1:B:171:ARG:NE	1.68	1.54
1:A:170:ASN:OD1	1:A:170:ASN:CG	1.65	1.34
1:A:65:ILE:HD12	1:A:66:PRO:HD2	1.19	1.11
1:A:87:THR:HG21	1:A:146:ARG:HH22	1.05	1.10
1:A:103:LYS:HD2	1:A:103:LYS:H	1.24	1.01
1:A:3:GLU:HG2	1:A:4:GLU:H	1.24	0.99
1:A:87:THR:HG21	1:A:146:ARG:NH2	1.84	0.91
1:A:152:ARG:HH11	1:B:135:ASN:HD21	1.16	0.91
1:B:85:LEU:HD21	1:B:153:ILE:HD11	1.53	0.91
1:A:22:PHE:O	1:A:25:THR:HB	1.73	0.88
1:B:171:ARG:CD	1:B:171:ARG:CZ	2.54	0.84
1:A:152:ARG:NH1	1:B:135:ASN:HD21	1.75	0.83
1:B:62:VAL:HG22	1:B:72:LYS:HB3	1.61	0.82
1:A:3:GLU:HG2	1:A:4:GLU:N	1.95	0.81
1:A:1:MET:SD	1:A:6:ASN:ND2	2.54	0.80
1:A:121:ASN:HD22	1:A:121:ASN:H	1.30	0.79
1:A:152:ARG:NH2	3:A:221:HOH:O	2.08	0.77
1:A:169:GLU:O	3:A:222:HOH:O	2.04	0.75
1:A:65:ILE:CD1	1:A:66:PRO:HD2	2.10	0.74
1:B:125:ARG:HG3	1:B:125:ARG:HH11	1.52	0.73
1:A:159:ILE:O	1:A:163:MET:HB2	1.89	0.73
1:B:120:ILE:H	1:B:120:ILE:HD12	1.53	0.73
1:A:152:ARG:NH1	1:B:135:ASN:ND2	2.37	0.71
1:B:120:ILE:O	1:B:124:MET:HG2	1.91	0.70
1:A:121:ASN:H	1:A:121:ASN:ND2	1.88	0.70
1:A:135:ASN:HD21	1:B:152:ARG:HD3	1.55	0.70
1:B:22:PHE:O	1:B:25:THR:HB	1.92	0.70
1:A:188:GLY:HA2	1:A:191:ARG:HE	1.57	0.69
1:A:141:ILE:HG23	1:B:141:ILE:HG23	1.76	0.67
1:B:43:LYS:HG2	1:B:44:ALA:N	2.09	0.67
1:B:85:LEU:CD2	1:B:153:ILE:HD11	2.25	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:THR:HG22	1:A:26:LYS:HD3	1.78	0.65
1:A:98:ALA:O	1:A:99:LYS:CB	2.44	0.63
1:B:159:ILE:O	1:B:163:MET:HB2	1.98	0.63
1:A:45:VAL:HG12	1:A:49:LEU:HD22	1.78	0.63
1:A:22:PHE:CE1	1:B:1:MET:HA	2.34	0.63
1:A:43:LYS:HG2	1:A:44:ALA:H	1.64	0.63
1:B:110:ALA:O	1:B:114:ILE:HG13	2.00	0.62
1:A:103:LYS:HD2	1:A:103:LYS:N	2.06	0.61
1:A:130:PHE:HD2	1:B:155:ILE:HD11	1.65	0.61
1:B:166:LEU:HB2	1:B:174:ILE:CD1	2.31	0.61
1:A:129:GLU:OE2	1:A:129:GLU:HA	1.99	0.61
1:A:121:ASN:HD22	1:A:121:ASN:N	1.92	0.61
1:A:3:GLU:CG	1:A:4:GLU:H	2.07	0.60
1:B:125:ARG:HG3	1:B:125:ARG:NH1	2.16	0.60
1:B:103:LYS:HE2	1:B:103:LYS:N	2.17	0.60
1:B:17:ARG:HD2	1:B:52:LEU:HD13	1.82	0.59
1:A:65:ILE:HD12	1:A:66:PRO:CD	2.13	0.58
1:B:166:LEU:HB2	1:B:174:ILE:HD11	1.86	0.57
1:A:169:GLU:O	1:A:170:ASN:HB3	2.05	0.57
1:A:124:MET:HB3	1:B:181:ILE:HD11	1.85	0.57
1:A:130:PHE:CD2	1:B:155:ILE:HD11	2.40	0.56
1:A:23:LEU:HD12	1:A:34:LEU:HD23	1.88	0.56
1:A:181:ILE:HD11	1:B:124:MET:HB3	1.88	0.55
1:A:135:ASN:ND2	1:B:152:ARG:HD3	2.21	0.54
1:A:69:ARG:HB2	1:A:70:PRO:CD	2.36	0.54
1:A:98:ALA:O	1:A:99:LYS:HB2	2.07	0.53
1:A:139:ARG:HD3	1:B:96:TYR:CE1	2.43	0.53
1:A:175:GLU:HA	1:A:175:GLU:OE1	2.08	0.53
1:B:65:ILE:O	1:B:66:PRO:O	2.27	0.53
1:A:124:MET:HB3	1:B:181:ILE:CD1	2.37	0.53
1:A:31:VAL:HG23	3:A:207:HOH:O	2.08	0.53
1:A:169:GLU:O	1:A:170:ASN:CB	2.57	0.52
1:B:178:PHE:CZ	1:B:194:LYS:HB2	2.45	0.52
1:A:178:PHE:CZ	1:A:194:LYS:HB2	2.46	0.51
1:A:103:LYS:CD	1:A:103:LYS:H	2.09	0.51
1:A:121:ASN:N	1:A:121:ASN:ND2	2.53	0.51
1:B:171:ARG:CG	1:B:171:ARG:NE	2.67	0.51
1:A:65:ILE:O	1:A:66:PRO:O	2.29	0.51
1:A:23:LEU:HD12	1:A:34:LEU:CD2	2.40	0.51
1:B:166:LEU:CB	1:B:174:ILE:CD1	2.89	0.51
1:A:135:ASN:HD21	1:B:152:ARG:CD	2.22	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PHE:CD1	1:B:1:MET:HG3	2.47	0.49
1:B:65:ILE:O	1:B:66:PRO:C	2.51	0.49
1:A:59:GLU:HG2	1:A:77:LYS:HA	1.95	0.48
1:A:65:ILE:O	1:A:66:PRO:C	2.51	0.48
1:B:101:VAL:O	1:B:102:ARG:HB2	2.14	0.48
1:A:187:PRO:O	1:A:191:ARG:HG3	2.13	0.47
1:B:196:LYS:HD2	1:B:196:LYS:HA	1.70	0.47
1:A:145:LYS:HB2	1:B:141:ILE:HG21	1.97	0.47
1:A:193:LEU:HA	1:A:193:LEU:HD23	1.68	0.47
1:B:103:LYS:HE2	1:B:103:LYS:H	1.80	0.47
1:B:166:LEU:CB	1:B:174:ILE:HD13	2.44	0.47
1:B:104:SER:OG	1:B:106:GLU:HG2	2.14	0.46
1:A:104:SER:HB2	1:A:105:PRO:HD2	1.98	0.46
1:A:135:ASN:ND2	1:B:152:ARG:HH11	2.12	0.46
1:B:164:ARG:O	1:B:165:ARG:C	2.53	0.46
1:A:30:PHE:CD1	1:A:71:ARG:HD3	2.51	0.45
1:B:121:ASN:ND2	1:B:121:ASN:H	2.14	0.45
1:A:181:ILE:CD1	1:B:124:MET:HB3	2.47	0.45
1:A:45:VAL:HG12	1:A:49:LEU:CD2	2.46	0.45
1:A:195:GLU:O	1:A:195:GLU:HG3	2.17	0.44
1:A:35:SER:O	1:A:39:GLY:N	2.50	0.44
1:B:170:ASN:ND2	1:B:173:ILE:HD11	2.33	0.44
1:A:119:PRO:HG2	1:A:122:VAL:HG23	1.99	0.44
1:B:170:ASN:HB2	1:B:173:ILE:HD11	1.99	0.43
1:B:120:ILE:CD1	1:B:120:ILE:H	2.25	0.43
1:A:166:LEU:C	1:A:168:GLU:H	2.22	0.43
1:B:43:LYS:HD2	3:B:213:HOH:O	2.18	0.43
1:A:111:LYS:O	1:A:115:LYS:HG2	2.19	0.43
1:B:149:GLU:CD	1:B:152:ARG:HH21	2.22	0.43
1:A:142:ILE:HD11	1:B:145:LYS:HE3	2.00	0.43
1:B:169:GLU:O	1:B:170:ASN:HB3	2.17	0.43
1:A:153:ILE:O	1:A:153:ILE:HG22	2.19	0.43
1:A:147:GLU:HB3	1:B:104:SER:HB3	2.01	0.43
1:B:171:ARG:HB2	1:B:171:ARG:NE	2.34	0.43
1:A:8:LEU:HD23	1:A:8:LEU:HA	1.88	0.43
1:B:89:THR:HB	1:B:157:THR:HG23	2.00	0.42
1:A:31:VAL:HG21	1:A:46:LEU:HD21	2.01	0.42
1:B:62:VAL:HG22	1:B:72:LYS:CB	2.40	0.42
1:A:120:ILE:O	1:A:124:MET:HG2	2.19	0.42
1:A:127:LEU:HA	1:A:127:LEU:HD13	1.69	0.42
1:A:30:PHE:HD2	1:A:33:GLU:OE2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:HA	1:A:148:LEU:HD12	1.88	0.42
1:B:109:GLN:O	1:B:112:GLU:HB3	2.20	0.42
1:A:1:MET:HE1	1:B:18:ARG:HB3	2.02	0.41
1:B:121:ASN:HD22	1:B:121:ASN:N	2.18	0.41
1:A:171:ARG:O	1:A:171:ARG:HD3	2.19	0.41
1:A:76:ILE:HG13	1:B:88:PRO:HA	2.02	0.41
1:B:127:LEU:HD13	1:B:127:LEU:HA	1.80	0.41
1:B:121:ASN:HD22	1:B:121:ASN:H	1.69	0.41
1:B:5:LEU:HA	1:B:5:LEU:HD23	1.81	0.41
1:B:178:PHE:HZ	1:B:194:LYS:HB2	1.86	0.41
1:A:22:PHE:CD1	1:B:1:MET:HA	2.57	0.40
1:B:135:ASN:HD22	1:B:135:ASN:HA	1.72	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	195/202 (96%)	177 (91%)	11 (6%)	7 (4%)	3	4
1	B	196/202 (97%)	181 (92%)	7 (4%)	8 (4%)	3	3
All	All	391/404 (97%)	358 (92%)	18 (5%)	15 (4%)	3	4

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	ARG
1	A	120	ILE
1	A	170	ASN
1	A	182	GLU
1	B	120	ILE
1	B	170	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	66	PRO
1	A	99	LYS
1	B	71	ARG
1	B	102	ARG
1	B	66	PRO
1	B	182	GLU
1	A	196	LYS
1	B	196	LYS
1	B	69	ARG

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	179/184 (97%)	151 (84%)	28 (16%)	2	4
1	B	180/184 (98%)	155 (86%)	25 (14%)	3	6
All	All	359/368 (98%)	306 (85%)	53 (15%)	3	5

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	ASN
1	A	7	ARG
1	A	10	ASP
1	A	12	LEU
1	A	43	LYS
1	A	49	LEU
1	A	52	LEU
1	A	71	ARG
1	A	78	LYS
1	A	85	LEU
1	A	86	LEU
1	A	103	LYS
1	A	106	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	112	GLU
1	A	121	ASN
1	A	127	LEU
1	A	141	ILE
1	A	143	GLU
1	A	148	LEU
1	A	171	ARG
1	A	173	ILE
1	A	174	ILE
1	A	179	ARG
1	A	181	ILE
1	A	192	SER
1	A	194	LYS
1	A	196	LYS
1	B	5	LEU
1	B	10	ASP
1	B	12	LEU
1	B	36	ARG
1	B	43	LYS
1	B	49	LEU
1	B	52	LEU
1	B	61	ARG
1	B	69	ARG
1	B	71	ARG
1	B	78	LYS
1	B	86	LEU
1	B	101	VAL
1	B	103	LYS
1	B	106	GLU
1	B	121	ASN
1	B	127	LEU
1	B	143	GLU
1	B	146	ARG
1	B	148	LEU
1	B	171	ARG
1	B	173	ILE
1	B	174	ILE
1	B	179	ARG
1	B	196	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	135	ASN
1	B	109	GLN
1	B	121	ASN
1	B	135	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	A	203	-	4,4,4	0.20	0	6,6,6	0.73	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	A	197/202 (97%)	0.13	8 (4%) 37 30	24, 32, 38, 43	5 (2%)
1	B	198/202 (98%)	0.12	12 (6%) 21 16	25, 32, 37, 39	0
All	All	395/404 (97%)	0.13	20 (5%) 28 22	24, 32, 37, 43	5 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	GLY	8.2
1	B	101	VAL	7.7
1	A	167	ALA	4.9
1	B	166	LEU	4.5
1	B	104	SER	4.0
1	A	163	MET	3.8
1	B	117	GLN	3.5
1	A	197	PHE	3.3
1	A	195	GLU	3.3
1	B	102	ARG	3.2
1	B	64	LYS	3.1
1	B	70	PRO	2.9
1	A	99	LYS	2.7
1	B	120	ILE	2.7
1	A	69	ARG	2.6
1	B	67	ARG	2.5
1	B	99	LYS	2.5
1	B	171	ARG	2.4
1	A	171	ARG	2.3
1	A	97	GLU	2.3

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](#)

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, 95th 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(\AA^2)	Q<0.9
2	SO4	A	203	5/5	0.96	0.11	61,62,63,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.