Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 02:49 PM JST

PDB ID	:	6JG9
Title	:	Crystal structure of AimR in complex with arbitrium peptide
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Deposited on	:	2019-02-13
Resolution	:	2.00 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

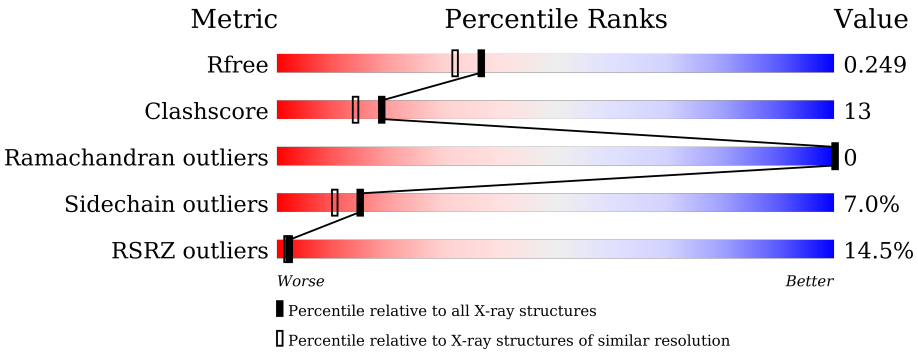
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 >=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 <=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	395	13% 78% 17%
1	B	395	16% 77% 18%
2	C	6	100%
2	D	6	83% 17%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6881 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 AimR transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3202	2045	533	603	21			
1	B	390	Total	C	N	O	S	0	0	0
			3193	2039	534	599	21			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP O64094
A	387	LEU	-	expression tag	UNP O64094
A	388	GLU	-	expression tag	UNP O64094
A	389	HIS	-	expression tag	UNP O64094
A	390	HIS	-	expression tag	UNP O64094
A	391	HIS	-	expression tag	UNP O64094
A	392	HIS	-	expression tag	UNP O64094
A	393	HIS	-	expression tag	UNP O64094
A	394	HIS	-	expression tag	UNP O64094
B	0	MET	-	initiating methionine	UNP O64094
B	387	LEU	-	expression tag	UNP O64094
B	388	GLU	-	expression tag	UNP O64094
B	389	HIS	-	expression tag	UNP O64094
B	390	HIS	-	expression tag	UNP O64094
B	391	HIS	-	expression tag	UNP O64094
B	392	HIS	-	expression tag	UNP O64094
B	393	HIS	-	expression tag	UNP O64094
B	394	HIS	-	expression tag	UNP O64094

- Molecule 2 is a protein called arbitrium peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	S	0	0	0
			40	23	9	7	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	6	Total	C	N	O	S	0	0	0
			40	23	9	7	1			

- Molecule 3 is water.

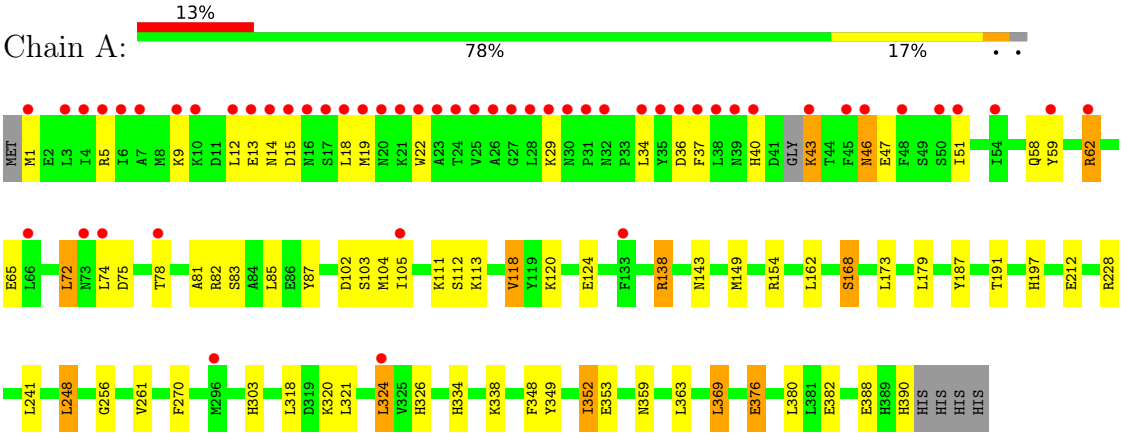
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	238	Total	O	0	0
			238	238		
3	C	8	Total	O	0	0
			8	8		
3	B	156	Total	O	0	0
			156	156		
3	D	4	Total	O	0	0
			4	4		

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.

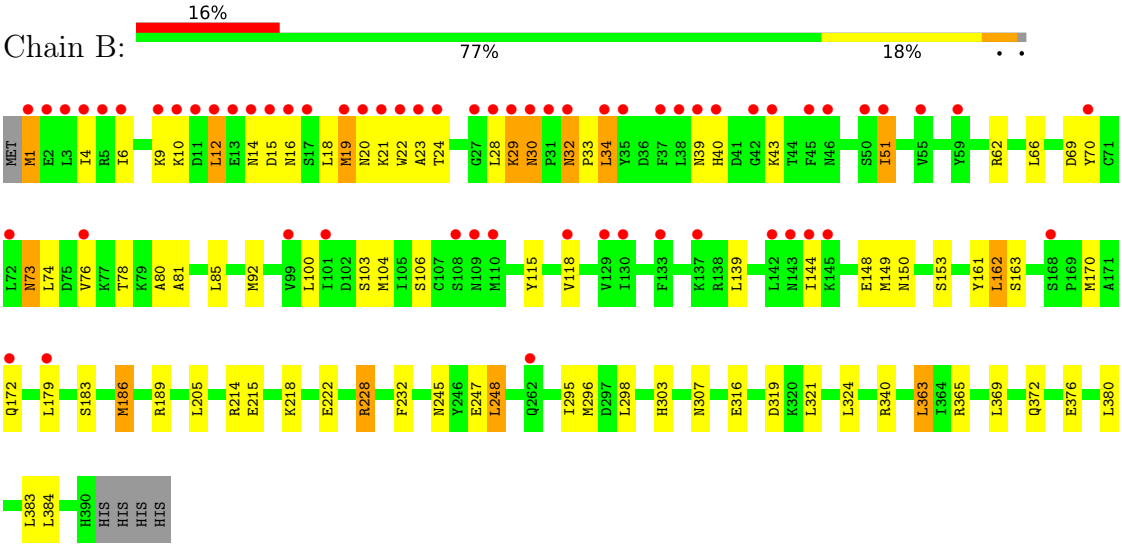
• Molecule 1: AimR transcriptional regulator

Chain A:



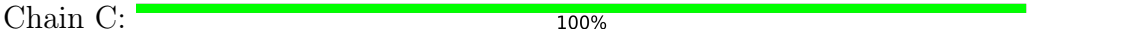
• Molecule 1: AimR transcriptional regulator

Chain B:



• Molecule 2: arbitrium peptide

Chain C:



There are no outlier residues recorded for this chain.

• Molecule 2: arbitrium peptide

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	120.93Å 214.00Å 33.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.12 – 2.00 46.12 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.12-2.00) 99.9 (46.12-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.65 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.14rc3_3206: ???)	Depositor
R, R_{free}	0.213 , 0.249 0.213 , 0.249	Depositor DCC
R_{free} test set	2973 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6881	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.48	0/3259	0.59	1/4384 (0.0%)
1	B	0.50	0/3250	0.64	2/4373 (0.0%)
2	C	0.47	0/40	0.76	0/50
2	D	0.54	0/40	0.92	0/50
All	All	0.49	0/6589	0.61	3/8857 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	369	LEU	CA-CB-CG	5.24	127.34	115.30
1	B	365	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	74	LEU	CA-CB-CG	5.00	126.80	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	3202	0	3193	71	0
1	B	3193	0	3186	98	0
2	C	40	0	42	0	0
2	D	40	0	42	1	0
3	A	238	0	0	39	0
3	B	156	0	0	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	8	0	0	0	0
3	D	4	0	0	0	0
All	All	6881	0	6463	169	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 13.

All (169) 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:320:LYS:HD3	3:A:405:HOH:O	1.35	1.24
1:A:9:LYS:HD2	3:A:498:HOH:O	1.15	1.23
1:A:1:MET:SD	3:A:498:HOH:O	2.00	1.19
1:B:12:LEU:HD22	3:B:402:HOH:O	1.40	1.18
1:B:16:ASN:HA	3:B:402:HOH:O	1.00	1.16
1:A:320:LYS:CD	3:A:405:HOH:O	1.91	1.11
1:A:320:LYS:NZ	3:A:405:HOH:O	1.87	1.07
1:A:19:MET:SD	3:A:600:HOH:O	2.14	1.03
1:A:87:TYR:HB2	3:A:410:HOH:O	1.56	1.03
1:B:73:ASN:HB3	3:B:416:HOH:O	1.57	1.02
1:B:92:MET:HE2	1:B:228:ARG:HG3	1.42	1.00
1:B:319:ASP:OD1	3:B:401:HOH:O	1.81	0.99
1:A:87:TYR:CB	3:A:410:HOH:O	2.11	0.98
1:A:87:TYR:HA	3:A:410:HOH:O	1.64	0.98
1:A:87:TYR:CA	3:A:410:HOH:O	2.12	0.98
1:B:1:MET:N	3:B:407:HOH:O	1.98	0.95
1:B:15:ASP:O	3:B:402:HOH:O	1.83	0.93
1:A:143:ASN:OD1	3:A:402:HOH:O	1.85	0.93
1:B:33:PRO:CB	3:B:403:HOH:O	2.16	0.93
1:A:382:GLU:OE1	3:A:404:HOH:O	1.87	0.93
1:B:33:PRO:CA	3:B:403:HOH:O	2.17	0.93
1:B:33:PRO:O	3:B:403:HOH:O	1.85	0.92
1:B:92:MET:CE	1:B:228:ARG:HG3	1.98	0.92
1:A:83:SER:OG	3:A:406:HOH:O	1.88	0.92
1:B:162:LEU:HA	1:B:170:MET:HE1	1.54	0.88
1:B:372:GLN:OE1	3:B:404:HOH:O	1.90	0.88
1:A:46:ASN:OD1	3:A:407:HOH:O	1.91	0.87
1:A:102:ASP:OD2	3:A:408:HOH:O	1.92	0.86
1:A:102:ASP:CB	3:A:408:HOH:O	2.24	0.86
1:A:1:MET:N	3:A:403:HOH:O	1.86	0.86
1:A:47:GLU:OE1	3:A:409:HOH:O	1.93	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ALA:HB2	3:B:427:HOH:O	1.76	0.85
1:B:69:ASP:OD2	3:B:405:HOH:O	1.93	0.85
1:B:33:PRO:HB3	3:B:403:HOH:O	1.75	0.85
1:A:65:GLU:OE2	3:A:411:HOH:O	1.96	0.83
1:A:349:TYR:OH	1:A:376:GLU:OE1	1.97	0.82
1:B:12:LEU:O	3:B:402:HOH:O	1.98	0.81
1:B:115:TYR:OH	1:B:148:GLU:HG2	1.80	0.81
1:B:33:PRO:C	3:B:403:HOH:O	2.18	0.79
1:B:186:MET:CE	1:B:189:ARG:HH21	1.96	0.79
1:B:215:GLU:OE2	3:B:408:HOH:O	2.01	0.79
1:B:92:MET:CE	1:B:228:ARG:CG	2.61	0.78
1:B:100:LEU:O	1:B:104:MET:HG3	1.84	0.78
1:B:186:MET:HE1	1:B:189:ARG:HH21	1.47	0.78
1:A:78:THR:HG23	1:A:81:ALA:H	1.48	0.77
1:B:30:ASN:O	1:B:30:ASN:ND2	2.19	0.75
1:B:34:LEU:HD12	3:B:427:HOH:O	1.87	0.74
1:B:30:ASN:HB2	3:B:413:HOH:O	1.86	0.74
1:A:124:GLU:OE1	1:A:138:ARG:NH2	2.20	0.73
1:B:92:MET:HE2	1:B:228:ARG:CG	2.17	0.73
1:B:40:HIS:HB2	1:B:43:LYS:HD3	1.71	0.72
1:B:118:VAL:HG22	1:B:149:MET:HE3	1.70	0.71
1:B:162:LEU:CA	1:B:170:MET:HE1	2.21	0.71
1:B:21:LYS:O	1:B:24:THR:OG1	2.08	0.71
1:B:19:MET:CE	1:B:34:LEU:HD13	2.22	0.70
1:A:118:VAL:HG22	1:A:149:MET:CE	2.22	0.70
1:B:247:GLU:OE1	3:B:409:HOH:O	2.09	0.69
1:B:1:MET:SD	3:B:532:HOH:O	2.51	0.68
1:B:12:LEU:CD2	3:B:402:HOH:O	2.16	0.68
1:B:307:ASN:OD1	1:B:340:ARG:NH2	2.18	0.67
1:A:75:ASP:O	1:A:78:THR:HG22	1.94	0.67
1:B:162:LEU:N	1:B:170:MET:CE	2.59	0.66
1:A:62:ARG:NH2	3:A:411:HOH:O	2.06	0.65
1:B:115:TYR:HA	1:B:149:MET:HE1	1.78	0.65
1:A:82:ARG:NH1	3:A:401:HOH:O	1.83	0.64
1:B:19:MET:HE1	1:B:34:LEU:HD13	1.80	0.63
1:B:4:ILE:HG22	3:B:405:HOH:O	1.98	0.63
1:B:92:MET:HE3	1:B:228:ARG:CG	2.27	0.63
1:A:65:GLU:CD	3:A:411:HOH:O	2.35	0.62
1:B:183:SER:N	3:B:410:HOH:O	2.32	0.61
1:A:187:TYR:CE2	3:A:410:HOH:O	2.51	0.61
1:A:102:ASP:HB2	3:A:408:HOH:O	1.94	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:GLN:CD	3:B:404:HOH:O	2.32	0.61
1:B:115:TYR:HA	1:B:149:MET:CE	2.31	0.60
1:A:261:VAL:HA	3:A:477:HOH:O	2.02	0.59
1:B:118:VAL:HG13	1:B:149:MET:HE2	1.83	0.59
1:B:23:ALA:CA	3:B:427:HOH:O	2.50	0.58
1:B:295:ILE:CD1	1:B:324:LEU:HD23	2.35	0.57
1:B:15:ASP:C	3:B:402:HOH:O	2.28	0.57
1:B:162:LEU:N	1:B:170:MET:HE2	2.20	0.56
1:B:295:ILE:HD13	1:B:324:LEU:HD23	1.87	0.56
1:A:241:LEU:HD13	1:A:248:LEU:HB3	1.87	0.56
1:B:92:MET:HE3	1:B:228:ARG:HG3	1.84	0.55
1:A:22:TRP:NE1	1:A:58:GLN:HG3	2.22	0.55
1:A:102:ASP:CG	3:A:408:HOH:O	2.36	0.55
1:B:78:THR:HG23	1:B:81:ALA:H	1.72	0.55
1:B:162:LEU:CA	1:B:170:MET:CE	2.85	0.55
1:A:22:TRP:HE1	1:A:58:GLN:HG3	1.71	0.54
1:A:191:THR:HG22	3:A:622:HOH:O	2.06	0.54
3:B:446:HOH:O	2:D:4:ARG:HD3	2.06	0.54
1:A:318:LEU:HD23	1:A:321:LEU:HD12	1.90	0.54
1:A:118:VAL:HG22	1:A:149:MET:HE1	1.90	0.54
1:A:353:GLU:HB2	1:B:383:LEU:HD13	1.90	0.53
1:B:139:LEU:HD13	1:B:153:SER:HB2	1.90	0.53
1:A:46:ASN:CB	3:A:407:HOH:O	2.57	0.53
1:A:320:LYS:CE	3:A:405:HOH:O	2.27	0.52
1:B:163:SER:OG	3:B:411:HOH:O	2.18	0.52
1:B:92:MET:HE3	1:B:228:ARG:HG2	1.92	0.52
1:B:144:ILE:CG2	1:B:150:ASN:OD1	2.58	0.52
1:B:186:MET:HE1	1:B:189:ARG:NH2	2.23	0.51
1:A:104:MET:HG2	1:A:112:SER:HB3	1.93	0.51
1:B:76:VAL:HG11	1:B:103:SER:HB3	1.92	0.51
1:B:92:MET:CE	1:B:228:ARG:HG2	2.41	0.49
1:B:186:MET:HE3	1:B:189:ARG:HH21	1.74	0.49
1:B:9:LYS:NZ	1:B:39:ASN:OD1	2.27	0.49
1:A:348:PHE:O	1:A:352:ILE:HG23	2.13	0.49
1:A:118:VAL:CG2	1:A:149:MET:HE3	2.44	0.48
1:B:115:TYR:OH	1:B:148:GLU:CG	2.58	0.48
1:B:92:MET:HE1	1:B:232:PHE:HE2	1.79	0.48
1:A:1:MET:CA	3:A:403:HOH:O	2.49	0.48
1:B:12:LEU:HD23	1:B:18:LEU:HD12	1.95	0.47
1:B:186:MET:HE3	1:B:189:ARG:HE	1.78	0.47
1:A:118:VAL:CG2	1:A:149:MET:CE	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:GLU:HG3	3:A:425:HOH:O	2.15	0.47
1:B:78:THR:HG23	1:B:80:ALA:N	2.29	0.47
1:B:1:MET:SD	1:B:6:ILE:HG12	2.55	0.46
1:A:256:GLY:HA3	1:A:270:PHE:CZ	2.50	0.46
1:B:30:ASN:C	3:B:413:HOH:O	2.53	0.46
1:B:62:ARG:O	1:B:66:LEU:HG	2.14	0.46
1:B:18:LEU:HA	1:B:21:LYS:HD2	1.99	0.45
1:B:295:ILE:HD11	1:B:324:LEU:HB3	1.99	0.45
1:A:1:MET:HA	3:A:403:HOH:O	2.16	0.45
1:A:303:HIS:HD2	3:A:489:HOH:O	1.98	0.45
1:B:316:GLU:OE2	3:B:412:HOH:O	2.21	0.45
1:A:1:MET:CE	3:A:498:HOH:O	2.48	0.45
1:B:29:LYS:HD2	1:B:29:LYS:N	2.32	0.45
1:A:12:LEU:HA	1:A:12:LEU:HD23	1.74	0.44
1:A:338:LYS:NZ	3:A:424:HOH:O	2.50	0.44
1:A:334:HIS:NE2	1:A:338:LYS:HE2	2.32	0.44
1:A:390:HIS:N	3:A:412:HOH:O	2.00	0.44
1:B:19:MET:SD	1:B:34:LEU:HD13	2.58	0.43
1:B:214:ARG:HD2	3:B:545:HOH:O	2.17	0.43
1:A:36:ASP:OD1	1:A:40:HIS:ND1	2.51	0.43
1:A:37:PHE:HA	1:A:43:LYS:HG2	2.01	0.43
1:A:187:TYR:HE2	3:A:410:HOH:O	1.96	0.43
1:B:144:ILE:HG22	1:B:150:ASN:OD1	2.19	0.43
1:A:22:TRP:HE1	1:A:58:GLN:CG	2.31	0.43
1:B:186:MET:CE	1:B:189:ARG:NH2	2.74	0.43
1:B:214:ARG:O	1:B:218:LYS:HG2	2.19	0.43
1:B:18:LEU:HD13	1:B:22:TRP:CZ2	2.54	0.42
1:B:78:THR:CG2	1:B:81:ALA:H	2.30	0.42
1:B:161:TYR:CB	1:B:170:MET:HE3	2.49	0.42
1:A:352:ILE:HG13	1:A:353:GLU:N	2.30	0.42
1:B:32:ASN:HB2	3:B:413:HOH:O	2.17	0.42
1:B:384:LEU:HD23	1:B:384:LEU:HA	1.87	0.42
1:A:15:ASP:HB3	1:A:18:LEU:HG	2.01	0.42
1:B:21:LYS:H	1:B:21:LYS:HG3	1.71	0.42
1:B:51:ILE:HD13	1:B:70:TYR:CE2	2.55	0.42
1:A:22:TRP:HE1	1:A:58:GLN:CD	2.23	0.41
1:B:16:ASN:CA	3:B:402:HOH:O	1.84	0.41
1:A:168:SER:HA	1:A:359:ASN:HD22	1.84	0.41
1:A:1:MET:HG2	1:A:5:ARG:NH2	2.35	0.41
1:B:51:ILE:H	1:B:51:ILE:HG13	1.50	0.41
1:A:14:ASN:C	3:A:422:HOH:O	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:LEU:HD12	1:B:363:LEU:HA	1.90	0.41
1:B:43:LYS:HB3	1:B:43:LYS:HE2	1.88	0.41
1:A:324:LEU:O	1:A:326:HIS:HD2	2.04	0.41
1:B:20:ASN:O	1:B:24:THR:HG23	2.20	0.41
1:B:245:ASN:CG	1:B:248:LEU:HB2	2.41	0.41
1:B:303:HIS:CD2	1:B:340:ARG:HH21	2.39	0.41
1:B:14:ASN:N	1:B:14:ASN:OD1	2.54	0.41
1:A:59:TYR:HB3	1:A:62:ARG:HG3	2.03	0.40
1:A:72:LEU:HA	1:A:72:LEU:HD12	1.87	0.40
1:A:105:ILE:CD1	1:A:120:LYS:HD2	2.51	0.40
1:A:197:HIS:HE1	3:A:610:HOH:O	2.04	0.40
1:B:298:LEU:HB2	1:B:321:LEU:HD21	2.02	0.40
1:A:9:LYS:O	1:A:13:GLU:HG3	2.22	0.40
1:A:154:ARG:HG2	1:A:173:LEU:HD11	2.04	0.40
1:B:222:GLU:O	1:B:222:GLU:HG3	2.20	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	385/395 (98%)	381 (99%)	4 (1%)	0	100	100
1	B	388/395 (98%)	381 (98%)	7 (2%)	0	100	100
2	C	4/6 (67%)	4 (100%)	0	0	100	100
2	D	4/6 (67%)	4 (100%)	0	0	100	100
All	All	781/802 (97%)	770 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	361/369 (98%)	335 (93%)	26 (7%)	14 9
1	B	358/369 (97%)	333 (93%)	25 (7%)	15 10
2	C	3/3 (100%)	3 (100%)	0	100 100
2	D	3/3 (100%)	3 (100%)	0	100 100
All	All	725/744 (97%)	674 (93%)	51 (7%)	15 10

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	34	LEU
1	A	43	LYS
1	A	46	ASN
1	A	51	ILE
1	A	62	ARG
1	A	72	LEU
1	A	74	LEU
1	A	85	LEU
1	A	103	SER
1	A	111	LYS
1	A	113	LYS
1	A	118	VAL
1	A	138	ARG
1	A	162	LEU
1	A	168	SER
1	A	179	LEU
1	A	228	ARG
1	A	248	LEU
1	A	324	LEU
1	A	352	ILE
1	A	363	LEU
1	A	369	LEU
1	A	376	GLU

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Mol	Chain	Res	Type
1	A	380	LEU
1	A	388	GLU
1	B	1	MET
1	B	10	LYS
1	B	12	LEU
1	B	19	MET
1	B	28	LEU
1	B	29	LYS
1	B	30	ASN
1	B	32	ASN
1	B	34	LEU
1	B	51	ILE
1	B	73	ASN
1	B	85	LEU
1	B	106	SER
1	B	162	LEU
1	B	172	GLN
1	B	179	LEU
1	B	186	MET
1	B	205	LEU
1	B	228	ARG
1	B	248	LEU
1	B	296	MET
1	B	363	LEU
1	B	369	LEU
1	B	376	GLU
1	B	380	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	HIS
1	A	326	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)

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^{th} 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	389/395 (98%)	0.98	53 (13%) 3 2	16, 37, 81, 109	0
1	B	390/395 (98%)	1.09	62 (15%) 1 1	22, 43, 84, 106	0
2	C	6/6 (100%)	0.83	0 100 100	20, 21, 25, 31	0
2	D	6/6 (100%)	0.90	0 100 100	23, 24, 32, 36	0
All	All	791/802 (98%)	1.03	115 (14%) 2 2	16, 39, 84, 109	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	TYR	11.6
1	A	14	ASN	6.7
1	B	28	LEU	6.2
1	B	99	VAL	5.8
1	B	40	HIS	5.7
1	A	9	LYS	5.4
1	B	34	LEU	5.4
1	B	29	LYS	5.4
1	B	37	PHE	5.3
1	A	39	ASN	5.2
1	B	45	PHE	5.0
1	A	29	LYS	4.8
1	B	3	LEU	4.8
1	B	38	LEU	4.7
1	B	23	ALA	4.6
1	A	37	PHE	4.5
1	A	21	LYS	4.5
1	B	51	ILE	4.5
1	B	39	ASN	4.4
1	A	13	GLU	4.3
1	B	20	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	38	LEU	4.3
1	A	15	ASP	4.3
1	A	54	ILE	4.2
1	A	59	TYR	4.2
1	B	15	ASP	4.1
1	B	137	LYS	3.9
1	A	18	LEU	3.8
1	B	22	TRP	3.8
1	B	1	MET	3.7
1	B	6	ILE	3.7
1	A	4	ILE	3.6
1	A	16	ASN	3.6
1	B	21	LYS	3.6
1	A	50	SER	3.6
1	B	133	PHE	3.6
1	A	7	ALA	3.6
1	B	30	ASN	3.6
1	A	20	ASN	3.5
1	A	32	ASN	3.5
1	B	16	ASN	3.5
1	B	35	TYR	3.5
1	A	1	MET	3.4
1	B	10	LYS	3.4
1	B	13	GLU	3.4
1	A	5	ARG	3.4
1	B	14	ASN	3.4
1	B	31	PRO	3.4
1	B	118	VAL	3.3
1	A	34	LEU	3.2
1	B	12	LEU	3.2
1	A	22	TRP	3.2
1	B	42	GLY	3.1
1	A	6	ILE	3.1
1	B	72	LEU	3.1
1	B	101	ILE	3.1
1	B	172	GLN	3.0
1	A	105	ILE	3.0
1	B	32	ASN	2.9
1	A	27	GLY	2.9
1	A	46	ASN	2.9
1	B	144	ILE	2.9
1	A	36	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	73	ASN	2.8
1	A	40	HIS	2.8
1	B	17	SER	2.8
1	A	25	VAL	2.8
1	A	23	ALA	2.8
1	B	27	GLY	2.7
1	B	145	LYS	2.7
1	B	11	ASP	2.7
1	A	30	ASN	2.7
1	A	3	LEU	2.7
1	B	108	SER	2.7
1	B	4	ILE	2.6
1	B	109	ASN	2.6
1	A	10	LYS	2.6
1	B	129	VAL	2.6
1	B	262	GLN	2.6
1	B	142	LEU	2.6
1	A	26	ALA	2.6
1	B	19	MET	2.6
1	A	28	LEU	2.5
1	A	43	LYS	2.5
1	B	9	LYS	2.5
1	B	143	ASN	2.5
1	B	43	LYS	2.5
1	B	46	ASN	2.5
1	A	133	PHE	2.5
1	A	19	MET	2.5
1	B	76	VAL	2.4
1	B	59	TYR	2.4
1	A	62	ARG	2.4
1	B	179	LEU	2.4
1	B	50	SER	2.4
1	B	55	VAL	2.4
1	A	48	PHE	2.3
1	B	110	MET	2.3
1	A	51	ILE	2.3
1	A	17	SER	2.3
1	B	5	ARG	2.3
1	A	45	PHE	2.2
1	A	78	THR	2.2
1	B	168	SER	2.2
1	B	2	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	66	LEU	2.2
1	B	70	TYR	2.1
1	A	31	PRO	2.1
1	B	130	ILE	2.1
1	A	24	THR	2.1
1	A	296	MET	2.1
1	B	24	THR	2.1
1	A	74	LEU	2.1
1	A	12	LEU	2.0
1	A	324	LEU	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.