



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:45 AM UTC

PDB ID : 6JG8 / pdb_00006jg8
Title : Crystal structure of AimR in complex with DNA
Authors : Guan, Z.Y.; Pei, K.; Zou, T.T.
Deposited on : 2019-02-13
Resolution : 2.10 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

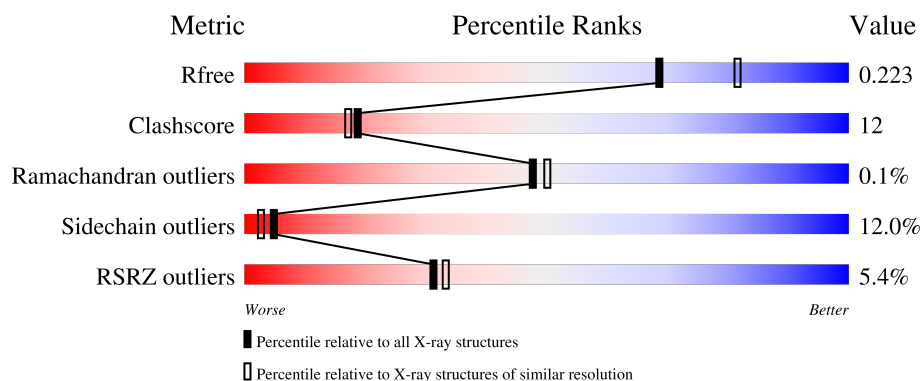
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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	395	 6% 68% 26% . .
1	B	395	 5% 70% 26% . .
2	C	31	 6% 55% 42% .
3	D	31	 3% 48% 48% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7913 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	386	Total	C	N	O	S	0	0	0
			3178	2029	528	600	21			
1	B	393	Total	C	N	O	S	0	1	0
			3251	2074	544	610	23			

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 DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	30	Total	C	N	O	P	0	0	0
			611	297	105	180	29			

- Molecule 3 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	30	Total	C	N	O	P	0	0	0
			616	297	111	178	30			

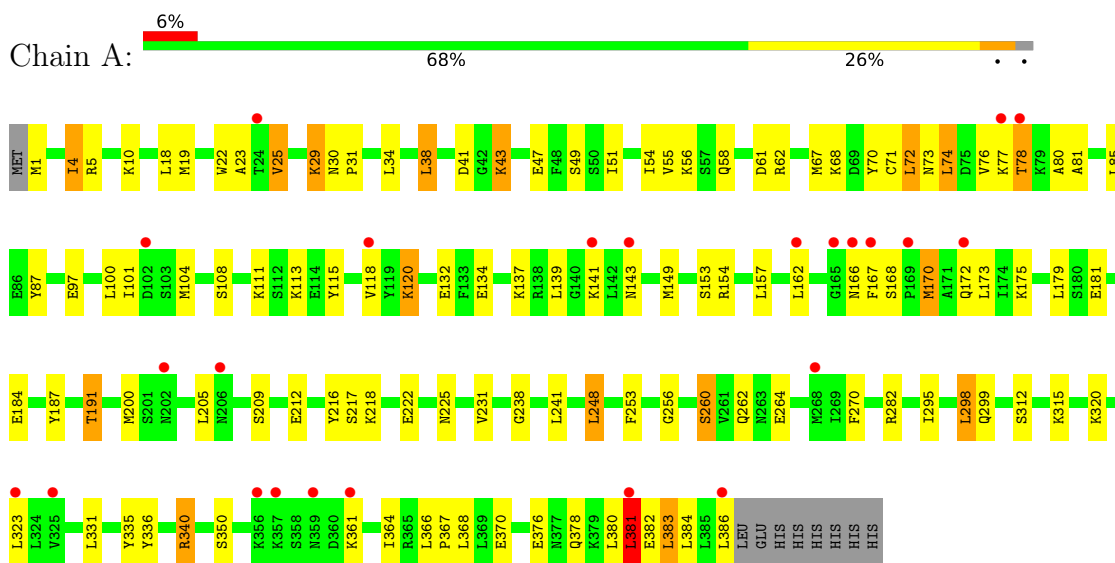
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	80	Total	O	0	0
			80	80		
4	B	161	Total	O	0	0
			161	161		
4	C	7	Total	O	0	0
			7	7		
4	D	9	Total	O	0	0
			9	9		

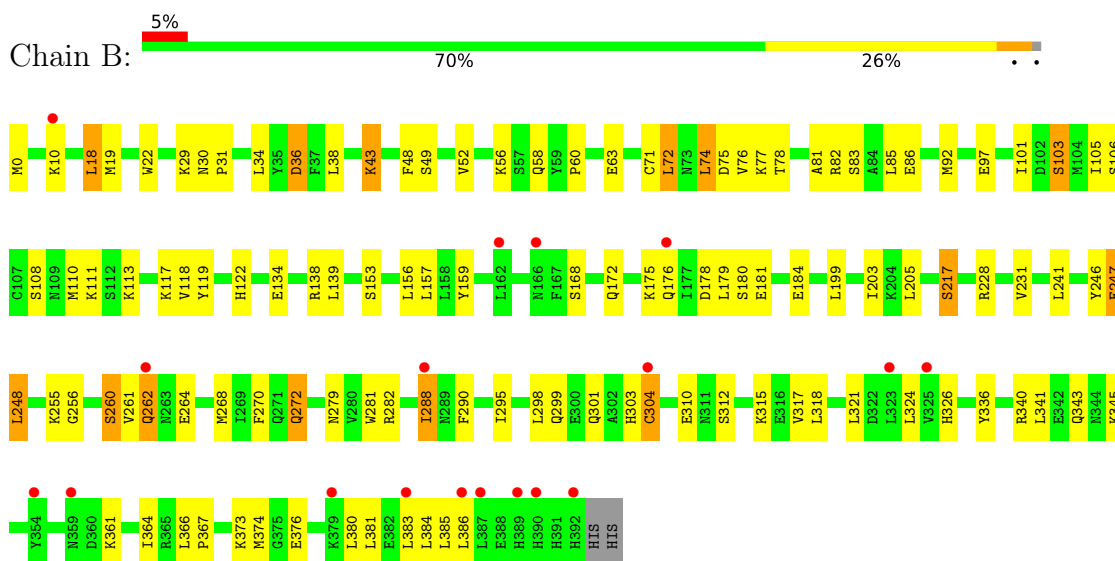
3 Residue-property plots

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.

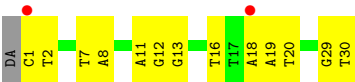
- Molecule 1: AimR transcriptional regulator



- Molecule 1: AimR transcriptional regulator



- Molecule 2: DNA (31-MER)



● Molecule 3: DNA (31-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	98.01Å 98.01Å 160.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.27 – 2.10 42.27 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.27-2.10) 99.6 (42.27-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.14rc3_3206: ???)	Depositor
R, R_{free}	0.210 , 0.222 0.211 , 0.223	Depositor DCC
R_{free} test set	4344 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7913	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.35	0/3235	0.56	1/4352 (0.0%)
1	B	0.41	1/3312 (0.0%)	0.58	0/4455
2	C	0.49	0/684	0.67	0/1054
3	D	0.47	0/691	0.70	0/1064
All	All	0.40	1/7922 (0.0%)	0.59	1/10925 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	CYS	CB-SG	5.64	1.99	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	LEU	CA-CB-CG	5.77	136.48	116.30

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	3178	0	3175	63	0
1	B	3251	0	3237	70	0
2	C	611	0	345	21	0
3	D	616	0	342	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	80	0	0	8	0
4	B	161	0	0	17	0
4	C	7	0	0	8	0
4	D	9	0	0	9	0
All	All	7913	0	7099	166	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 12.

All (166) 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:82:ARG:NE	4:B:401:HOH:O	1.74	1.07
3:D:24:DA:N7	4:D:101:HOH:O	1.86	1.06
1:B:176:GLN:OE1	4:B:402:HOH:O	1.75	1.04
1:B:82:ARG:NH2	4:B:401:HOH:O	1.93	0.99
2:C:18:DA:C1'	4:C:101:HOH:O	2.16	0.93
1:A:134:GLU:OE2	4:A:401:HOH:O	1.87	0.92
1:B:184:GLU:OE1	4:B:403:HOH:O	1.87	0.92
1:A:22:TRP:HE1	1:A:58:GLN:HG3	1.36	0.89
2:C:18:DA:N3	4:C:101:HOH:O	2.06	0.88
1:B:181:GLU:OE1	4:B:405:HOH:O	1.92	0.87
2:C:18:DA:H2''	4:C:101:HOH:O	1.76	0.84
3:D:9:DT:OP2	4:D:102:HOH:O	1.95	0.82
2:C:18:DA:C2'	4:C:101:HOH:O	2.27	0.80
2:C:30:DT:O4	3:D:1:DA:N6	2.13	0.79
2:C:1:DC:H2''	2:C:2:DT:H5''	1.63	0.79
2:C:18:DA:H1'	4:C:101:HOH:O	1.78	0.77
1:B:312:SER:OG	4:B:407:HOH:O	2.00	0.77
1:B:376:GLU:OE1	4:B:409:HOH:O	2.02	0.77
3:D:8:DG:OP2	4:D:103:HOH:O	2.03	0.77
1:B:71:CYS:HA	1:B:74:LEU:HD22	1.67	0.76
1:B:159:TYR:OH	4:B:408:HOH:O	2.01	0.76
1:A:256:GLY:O	1:A:260:SER:OG	2.05	0.73
1:B:111:LYS:HE3	4:D:103:HOH:O	1.87	0.73
1:B:117:LYS:NZ	4:B:406:HOH:O	1.96	0.73
1:A:78:THR:HG23	1:A:80:ALA:H	1.54	0.72
2:C:18:DA:C4	4:C:101:HOH:O	2.40	0.72
1:B:77:LYS:NZ	1:B:108:SER:OG	2.24	0.71
2:C:13:DG:H8	4:C:102:HOH:O	1.73	0.70
1:A:181:GLU:OE1	4:A:402:HOH:O	2.10	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:29:DG:H2''	2:C:30:DT:H71	1.72	0.70
1:A:139:LEU:HD13	1:A:153:SER:HB2	1.74	0.68
1:A:22:TRP:NE1	1:A:58:GLN:HG3	2.06	0.68
1:B:75:ASP:O	1:B:78:THR:HG22	1.93	0.67
1:A:71:CYS:HA	1:A:74:LEU:HD22	1.76	0.66
1:B:340:ARG:O	1:B:343:GLN:NE2	2.27	0.66
2:C:7:DT:H2''	2:C:8:DA:H5''	1.77	0.66
1:B:78:THR:OG1	4:B:410:HOH:O	2.08	0.66
3:D:24:DA:C5	4:D:101:HOH:O	2.37	0.66
1:A:154:ARG:HG2	1:A:173:LEU:HD11	1.79	0.65
1:B:60:PRO:O	4:B:411:HOH:O	2.13	0.65
1:B:138:ARG:NH1	4:B:415:HOH:O	2.29	0.65
1:B:217:SER:OG	4:B:413:HOH:O	2.15	0.65
1:A:166:ASN:O	1:A:168:SER:N	2.27	0.65
1:A:120:LYS:NZ	4:A:405:HOH:O	2.31	0.64
1:B:138:ARG:O	4:B:412:HOH:O	2.15	0.64
1:A:370:GLU:OE1	4:A:403:HOH:O	2.14	0.64
2:C:16:DT:H5'	2:C:16:DT:H6	1.62	0.63
3:D:24:DA:N6	4:D:101:HOH:O	2.14	0.63
1:B:255:LYS:NZ	4:B:404:HOH:O	1.89	0.62
2:C:19:DA:H1'	2:C:20:DT:H5'	1.81	0.62
1:A:101:ILE:HG21	1:A:120:LYS:HE2	1.81	0.61
1:B:30:ASN:HD21	2:C:30:DT:H71	1.66	0.61
3:D:30:DG:H5'	3:D:30:DG:H8	1.64	0.61
1:A:22:TRP:HE1	1:A:58:GLN:CG	2.10	0.61
1:B:178:ASP:OD1	1:B:180:SER:OG	2.18	0.59
1:B:262:GLN:CD	1:B:262:GLN:H	2.10	0.59
1:B:256:GLY:O	1:B:260:SER:OG	2.20	0.58
1:A:23:ALA:HB2	1:A:31:PRO:HB3	1.86	0.58
1:A:187:TYR:O	1:A:191:THR:HG23	2.03	0.58
1:B:336:TYR:CE1	1:B:366:LEU:HB3	2.39	0.58
1:A:231:VAL:HG13	1:A:270:PHE:HE2	1.69	0.57
1:B:22:TRP:HE1	1:B:58:GLN:CG	2.18	0.57
2:C:16:DT:H5'	2:C:16:DT:C6	2.39	0.57
1:A:364:ILE:O	1:A:367:PRO:HD2	2.05	0.57
1:B:36:ASP:HB3	1:B:43:LYS:HG3	1.87	0.56
1:A:43:LYS:HD3	4:D:107:HOH:O	2.04	0.56
1:B:364:ILE:O	1:B:367:PRO:HD2	2.06	0.56
1:A:115:TYR:CE2	1:A:149:MET:HE3	2.42	0.55
1:B:82:ARG:CZ	4:B:401:HOH:O	2.10	0.55
1:B:288:ILE:HD11	1:B:290:PHE:CD1	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:LEU:HD23	1:B:321:LEU:HD12	1.88	0.55
1:A:61:ASP:OD1	1:A:262:GLN:NE2	2.40	0.55
1:A:47:GLU:OE1	4:A:404:HOH:O	2.17	0.55
1:A:378:GLN:HA	1:A:381:LEU:HD22	1.89	0.53
1:A:162:LEU:HD23	1:A:170:MET:HE1	1.89	0.53
1:A:1:MET:N	4:A:406:HOH:O	2.34	0.53
1:B:97:GLU:O	1:B:101:ILE:HG13	2.09	0.53
1:B:288:ILE:HD11	1:B:290:PHE:CE1	2.44	0.53
1:B:261:VAL:HG23	1:B:262:GLN:HG3	1.91	0.53
1:A:111:LYS:NZ	1:A:184:GLU:OE2	2.38	0.52
1:B:139:LEU:HD13	1:B:153:SER:HB2	1.91	0.52
1:A:76:VAL:HB	1:A:104:MET:HG2	1.91	0.52
1:A:378:GLN:NE2	1:A:382:GLU:HG3	2.24	0.52
1:B:241:LEU:HD13	1:B:248:LEU:HB3	1.92	0.52
1:A:231:VAL:HG13	1:A:270:PHE:CE2	2.44	0.51
1:A:335:TYR:CD2	1:A:350:SER:HB3	2.45	0.51
3:D:24:DA:C6	4:D:101:HOH:O	2.55	0.51
1:B:77:LYS:HE3	3:D:9:DT:OP1	2.10	0.51
1:A:34:LEU:O	1:A:38:LEU:HD22	2.11	0.51
1:B:86:GLU:OE2	1:B:119:TYR:OH	2.26	0.51
1:A:336:TYR:CE1	1:A:366:LEU:HB3	2.46	0.50
1:B:78:THR:HG23	1:B:81:ALA:H	1.75	0.50
1:A:295:ILE:O	1:A:299:GLN:HG3	2.12	0.50
1:A:383:LEU:HB3	1:B:384:LEU:HD21	1.94	0.49
1:B:92:MET:HE2	1:B:228:ARG:HG3	1.95	0.49
1:A:241:LEU:HD13	1:A:248:LEU:HB3	1.94	0.49
1:B:324:LEU:O	1:B:326:HIS:HD2	1.96	0.49
1:A:368:LEU:HD22	1:A:381:LEU:HB2	1.95	0.48
1:A:376:GLU:HG2	1:B:380:LEU:HD11	1.95	0.48
1:B:10:LYS:HE2	4:B:437:HOH:O	2.13	0.48
3:D:30:DG:H8	3:D:30:DG:C5'	2.26	0.48
1:A:4:ILE:HD12	1:A:51:ILE:HD11	1.95	0.48
1:A:218:LYS:O	1:A:222:GLU:HG3	2.14	0.48
1:B:30:ASN:HD21	2:C:30:DT:C7	2.25	0.47
1:B:56:LYS:HZ2	1:B:63:GLU:CD	2.22	0.47
3:D:3:DT:H2''	3:D:4:DA:C8	2.49	0.47
1:B:279:ASN:ND2	1:B:303:HIS:HB3	2.29	0.47
1:B:315:LYS:HG3	1:B:341:LEU:HD21	1.96	0.47
1:A:30:ASN:OD1	1:A:30:ASN:C	2.56	0.47
1:A:78:THR:HG22	1:A:81:ALA:H	1.80	0.47
3:D:1:DA:H2''	3:D:2:DC:C6	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:TYR:O	1:A:74:LEU:HD13	2.14	0.46
1:B:247:GLU:H	1:B:247:GLU:CD	2.23	0.46
1:B:345:LYS:HE3	1:B:374:MET:HE2	1.98	0.46
1:A:366:LEU:HB2	1:A:367:PRO:HD3	1.97	0.46
1:A:315:LYS:HE3	1:A:315:LYS:HB2	1.62	0.45
1:A:68:LYS:O	1:A:72:LEU:HB2	2.16	0.45
2:C:12:DG:H2''	4:C:102:HOH:O	2.16	0.45
1:A:25:VAL:HG11	1:A:54:ILE:HA	1.99	0.45
1:B:288:ILE:HD13	1:B:301:GLN:HG2	1.98	0.45
1:B:199:LEU:O	1:B:203:ILE:HG13	2.17	0.45
1:B:298:LEU:HD22	1:B:317:VAL:HG13	1.98	0.45
1:A:67:MET:HG3	1:A:87:TYR:OH	2.17	0.45
1:B:110:MET:HE1	1:B:113:LYS:HE3	1.99	0.45
3:D:22:DA:N6	4:D:104:HOH:O	2.24	0.44
1:B:122:HIS:HB2	1:B:156:LEU:HD22	1.99	0.44
2:C:1:DC:H2'	2:C:2:DT:H72	2.00	0.44
3:D:22:DA:H2''	3:D:23:DT:O5'	2.17	0.44
1:A:200:MET:HG2	1:A:216:TYR:CE1	2.52	0.44
1:A:97:GLU:O	1:A:101:ILE:HG13	2.17	0.44
1:A:100:LEU:O	1:A:104:MET:HG3	2.17	0.44
1:B:172:GLN:OE1	1:B:176:GLN:NE2	2.49	0.44
3:D:13:DT:H2''	3:D:14:DA:C8	2.53	0.44
1:B:295:ILE:O	1:B:299:GLN:HG3	2.18	0.44
1:A:29:LYS:HD3	3:D:28:DA:OP1	2.17	0.44
1:B:52:VAL:HG12	1:B:56:LYS:HD2	1.99	0.44
1:A:5:ARG:NH1	1:A:41:ASP:HA	2.33	0.43
1:B:366:LEU:HB2	1:B:367:PRO:HD3	1.99	0.43
1:A:378:GLN:HA	1:A:381:LEU:CD2	2.48	0.43
1:B:48:PHE:HB2	1:B:83:SER:HB3	1.99	0.43
1:B:268[B]:MET:O	1:B:272:GLN:HG2	2.17	0.43
3:D:9:DT:H1'	3:D:10:DT:H5'	2.00	0.43
2:C:11:DA:C2	3:D:21:DA:C2	3.06	0.43
1:A:56:LYS:HD2	1:A:225:ASN:ND2	2.33	0.43
1:B:256:GLY:HA3	1:B:270:PHE:CZ	2.54	0.43
3:D:30:DG:C5'	3:D:30:DG:C8	3.01	0.43
1:A:78:THR:HG23	1:A:80:ALA:N	2.29	0.42
1:A:200:MET:HG2	1:A:216:TYR:CZ	2.54	0.42
1:A:282:ARG:NH1	4:A:415:HOH:O	2.52	0.42
3:D:30:DG:H5'	3:D:30:DG:C8	2.49	0.42
1:A:115:TYR:CD2	1:A:149:MET:HE3	2.55	0.42
1:A:191:THR:HG22	4:A:478:HOH:O	2.17	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:TRP:HE1	1:B:58:GLN:HG3	1.83	0.42
1:B:76:VAL:HG11	1:B:103:SER:HB3	2.01	0.42
1:A:340:ARG:HD3	1:A:370:GLU:OE2	2.19	0.42
1:B:72:LEU:HD12	1:B:72:LEU:HA	1.72	0.42
1:B:10:LYS:HE2	1:B:10:LYS:HB2	1.58	0.42
1:B:246:TYR:HB2	1:B:281:TRP:CD2	2.54	0.42
1:A:298:LEU:HD11	1:A:320:LYS:HE2	2.02	0.42
2:C:7:DT:H2''	2:C:8:DA:C5'	2.48	0.41
2:C:7:DT:C2'	2:C:8:DA:H5''	2.49	0.41
1:A:175:LYS:HE3	1:A:175:LYS:HB2	1.82	0.41
1:B:18:LEU:HD12	1:B:18:LEU:HA	1.76	0.40
1:B:31:PRO:O	1:B:34:LEU:HB2	2.21	0.40
1:B:30:ASN:HB2	1:B:31:PRO:HD2	2.03	0.40
1:A:238:GLY:HA3	1:A:253:PHE:CE1	2.57	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	384/395 (97%)	369 (96%)	14 (4%)	1 (0%)	36	36
1	B	392/395 (99%)	383 (98%)	9 (2%)	0	100	100
All	All	776/790 (98%)	752 (97%)	23 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	PHE

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	359/369 (97%)	311 (87%)	48 (13%)	4	2
1	B	367/369 (100%)	328 (89%)	39 (11%)	6	4
All	All	726/738 (98%)	639 (88%)	87 (12%)	5	3

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	10	LYS
1	A	18	LEU
1	A	19	MET
1	A	25	VAL
1	A	29	LYS
1	A	38	LEU
1	A	43	LYS
1	A	49	SER
1	A	55	VAL
1	A	62	ARG
1	A	72	LEU
1	A	73	ASN
1	A	74	LEU
1	A	77	LYS
1	A	78	THR
1	A	85	LEU
1	A	108	SER
1	A	113	LYS
1	A	118	VAL
1	A	120	LYS
1	A	132	GLU
1	A	137	LYS
1	A	141	LYS
1	A	143	ASN
1	A	157	LEU
1	A	170	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	172	GLN
1	A	179	LEU
1	A	191	THR
1	A	205	LEU
1	A	209	SER
1	A	212	GLU
1	A	217	SER
1	A	248	LEU
1	A	260	SER
1	A	264	GLU
1	A	298	LEU
1	A	312	SER
1	A	323	LEU
1	A	331	LEU
1	A	340	ARG
1	A	361	LYS
1	A	380	LEU
1	A	381	LEU
1	A	383	LEU
1	A	384	LEU
1	A	386	LEU
1	B	0	MET
1	B	18	LEU
1	B	19	MET
1	B	29	LYS
1	B	36	ASP
1	B	38	LEU
1	B	43	LYS
1	B	49	SER
1	B	72	LEU
1	B	74	LEU
1	B	85	LEU
1	B	103	SER
1	B	105	ILE
1	B	106	SER
1	B	118	VAL
1	B	134	GLU
1	B	157	LEU
1	B	168	SER
1	B	175	LYS
1	B	179	LEU
1	B	205	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	217	SER
1	B	231	VAL
1	B	247	GLU
1	B	248	LEU
1	B	260	SER
1	B	262	GLN
1	B	264	GLU
1	B	272	GLN
1	B	282	ARG
1	B	288	ILE
1	B	304	CYS
1	B	310	GLU
1	B	361	LYS
1	B	373	LYS
1	B	381	LEU
1	B	383	LEU
1	B	385	LEU
1	B	386	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	176	GLN
1	A	193	GLN
1	A	271	GLN
1	A	299	GLN
1	A	329	ASN
1	B	30	ASN
1	B	32	ASN
1	B	160	HIS
1	B	193	GLN
1	B	197	HIS
1	B	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 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, 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	386/395 (97%)	0.61	24 (6%) 26 28	43, 58, 88, 114	0
1	B	393/395 (99%)	0.55	18 (4%) 37 39	25, 53, 85, 119	1 (0%)
2	C	30/31 (96%)	0.64	2 (6%) 24 25	50, 76, 102, 114	0
3	D	30/31 (96%)	0.66	1 (3%) 49 51	56, 77, 103, 104	0
All	All	839/852 (98%)	0.59	45 (5%) 31 33	25, 56, 92, 119	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	PHE	4.9
1	A	386	LEU	4.4
1	B	386	LEU	4.3
1	B	389	HIS	4.1
1	B	325	VAL	3.7
1	B	304	CYS	3.6
1	A	162	LEU	3.5
1	A	359	ASN	3.3
1	B	392	HIS	3.3
1	A	356	LYS	3.1
1	B	390	HIS	3.0
1	A	24	THR	2.9
1	B	288	ILE	2.8
1	A	361	LYS	2.8
1	B	162	LEU	2.8
1	A	381	LEU	2.8
1	A	323	LEU	2.8
1	A	169	PRO	2.7
1	A	357	LYS	2.7
1	B	323	LEU	2.6
1	A	206	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	268	MET	2.6
3	D	17	DA	2.6
1	A	78	THR	2.5
1	B	359	ASN	2.5
1	A	102	ASP	2.5
1	B	262	GLN	2.4
1	A	172	GLN	2.4
1	A	325	VAL	2.4
1	B	387	LEU	2.3
2	C	1	DC	2.3
1	B	383	LEU	2.3
1	B	10	LYS	2.3
1	B	176	GLN	2.2
1	A	141	LYS	2.2
2	C	18	DA	2.2
1	B	354	TYR	2.2
1	A	202	ASN	2.1
1	A	165	GLY	2.1
1	A	77	LYS	2.1
1	A	166	ASN	2.1
1	B	379	LYS	2.1
1	A	118	VAL	2.0
1	A	143	ASN	2.0
1	B	166	ASN	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 oligosaccharides 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.