Full wwPDB X-ray Structure Validation Report ⓘ

Jan 13, 2024 – 10:46 pm GMT

PDB ID	:	6SDG
Title	:	Crystal structure of the DNA binding domain of M. polymorpha Auxin Response Factor 2 (MpARF2) in complex with High Affinity DNA
Authors	:	Crespo, I.; Weijers, D.; Boer, D.R.
Deposited on	:	2019-07-27
Resolution	:	2.96 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:

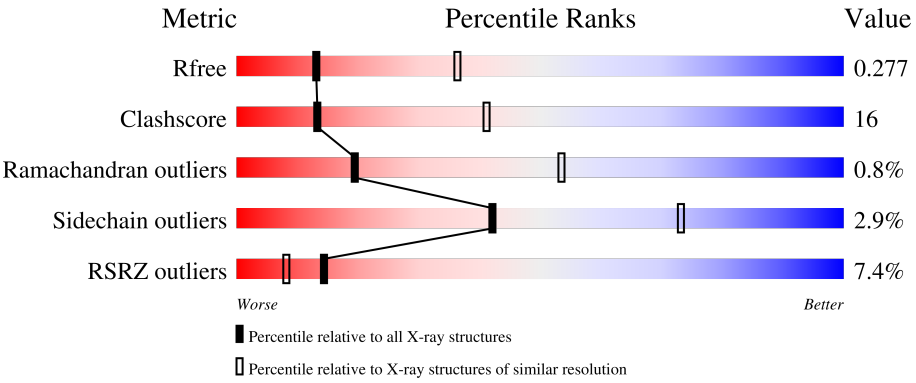
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.96 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	366	6% 56% 30% · 13%
1	B	366	8% 56% 28% · 14%
2	C	22	14% 73% 14%
3	D	22	27% 50% 23%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5890 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 Auxin response factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2511	1579	455	466	11			
1	B	314	Total	C	N	O	S	0	0	0
			2476	1558	449	458	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	GLY	-	expression tag	UNP A0A0K2QVG1
A	360	ASN	-	expression tag	UNP A0A0K2QVG1
A	361	SER	-	expression tag	UNP A0A0K2QVG1
A	362	TYR	-	expression tag	UNP A0A0K2QVG1
A	363	SER	-	expression tag	UNP A0A0K2QVG1
A	364	GLN	-	expression tag	UNP A0A0K2QVG1
A	365	SER	-	expression tag	UNP A0A0K2QVG1
A	366	MET	-	expression tag	UNP A0A0K2QVG1
B	359	GLY	-	expression tag	UNP A0A0K2QVG1
B	360	ASN	-	expression tag	UNP A0A0K2QVG1
B	361	SER	-	expression tag	UNP A0A0K2QVG1
B	362	TYR	-	expression tag	UNP A0A0K2QVG1
B	363	SER	-	expression tag	UNP A0A0K2QVG1
B	364	GLN	-	expression tag	UNP A0A0K2QVG1
B	365	SER	-	expression tag	UNP A0A0K2QVG1
B	366	MET	-	expression tag	UNP A0A0K2QVG1

- Molecule 2 is a DNA chain called 21-7_A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	21	Total	C	N	O	P	0	3	0
			454	215	83	134	22			

- Molecule 3 is a DNA chain called 21-7_B.

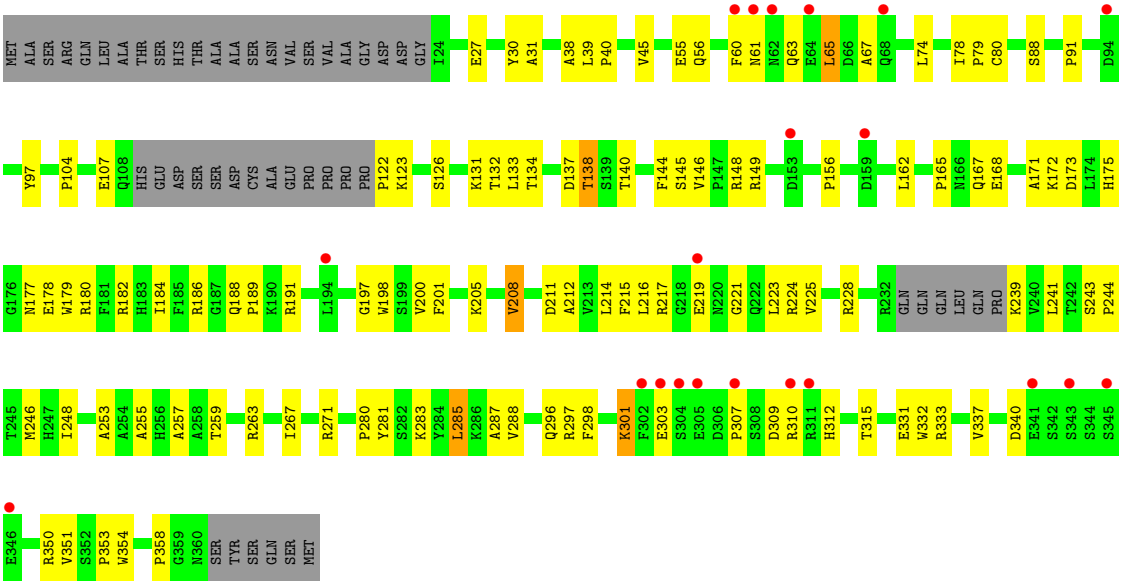
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	21	449	214	83	131	21	0	2	0

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.

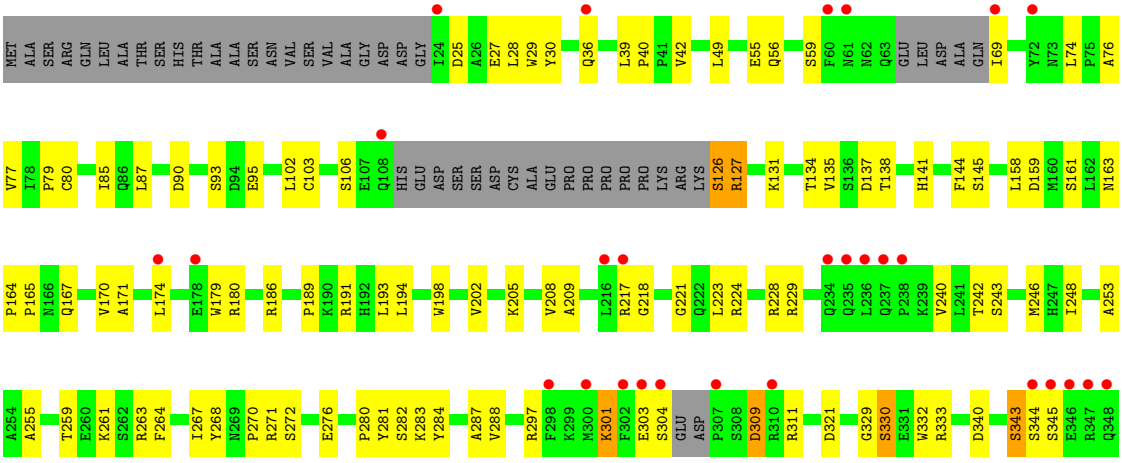
• Molecule 1: Auxin response factor

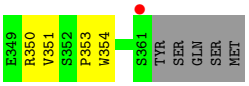
Chain A:



• Molecule 1: Auxin response factor

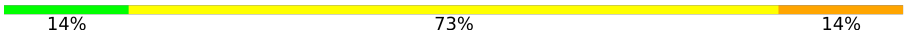
Chain B:

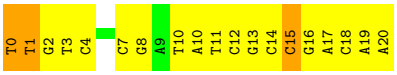




• Molecule 2: 21-7_A

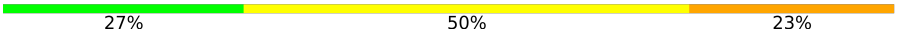
Chain C:

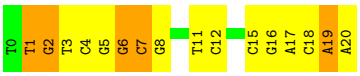




• Molecule 3: 21-7_B

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.77Å 79.36Å 79.77Å 90.00° 116.93° 90.00°	Depositor
Resolution (Å)	29.20 – 2.96 29.20 – 2.96	Depositor EDS
% Data completeness (in resolution range)	73.5 (29.20-2.96) 74.3 (29.20-2.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.215 , 0.278 0.215 , 0.277	Depositor DCC
R_{free} test set	768 reflections (5.48%)	wwPDB-VP
Wilson B-factor (Å^2)	101.1	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 53.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h+k-l,-l,-k 0.000 for -h-k-l,l,k 0.077 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5890	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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	0.65	0/2575	0.82	1/3495 (0.0%)
1	B	0.62	1/2539 (0.0%)	0.77	0/3447
2	C	1.17	3/547 (0.5%)	1.27	5/840 (0.6%)
3	D	1.32	5/525 (1.0%)	1.23	2/806 (0.2%)
All	All	0.77	9/6186 (0.1%)	0.90	8/8588 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	DT	C1'-N1	-7.39	1.36	1.47
3	D	7	DC	C3'-O3'	6.83	1.52	1.44
3	D	1	DT	C1'-N1	-6.17	1.38	1.47
3	D	19	DA	C3'-O3'	-5.74	1.36	1.44
3	D	1	DT	C4-O4	-5.56	1.18	1.23
2	C	10[B]	DA	O3'-P	-5.52	1.54	1.61
3	D	6	DG	C3'-O3'	5.48	1.51	1.44
1	B	351	VAL	C-N	5.12	1.45	1.34
2	C	12	DC	C1'-N1	5.04	1.55	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2	DG	O4'-C1'-N9	6.77	112.74	108.00
2	C	0	DT	N3-C4-O4	5.33	123.10	119.90
2	C	11[A]	DT	N3-C4-O4	5.25	123.05	119.90
2	C	11[B]	DT	N3-C4-O4	5.25	123.05	119.90
1	A	285	LEU	CA-CB-CG	-5.16	103.43	115.30
2	C	10[B]	DA	OP2-P-O3'	5.15	116.53	105.20
3	D	1	DT	C5-C4-O4	-5.10	121.33	124.90
2	C	15	DC	O4'-C4'-C3'	-5.02	102.49	104.50

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	2511	0	2465	77	0
1	B	2476	0	2429	82	0
2	C	454	0	238	20	0
3	D	449	0	240	20	0
All	All	5890	0	5372	182	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 16.

All (182) 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:297:ARG:NH2	1:B:340:ASP:OD2	2.07	0.86
3:D:17:DA:H5"	3:D:17:DA:H8	1.42	0.83
1:A:301:LYS:HD3	1:A:301:LYS:H	1.44	0.82
1:B:25:ASP:OD1	1:B:224:ARG:NH1	2.13	0.81
1:A:297:ARG:HG2	1:A:315:THR:HG22	1.63	0.79
1:B:141:HIS:NE2	3:D:6:DG:O6	2.17	0.78
1:B:127:ARG:HD2	1:B:217:ARG:HG2	1.67	0.77
1:B:27:GLU:OE2	1:B:126:SER:N	2.18	0.76
1:B:243:SER:HA	1:B:246:MET:HE2	1.67	0.75
3:D:17:DA:H5"	3:D:17:DA:C8	2.22	0.75
1:A:287:ALA:HB1	1:A:353:PRO:HB2	1.69	0.73
1:B:141:HIS:HD2	2:C:14:DC:H41	1.39	0.71
1:B:301:LYS:HD3	1:B:301:LYS:H	1.56	0.70
1:A:297:ARG:NH1	1:A:340:ASP:OD2	2.25	0.69
1:B:56:GLN:NE2	1:B:267:ILE:O	2.24	0.69
1:B:301:LYS:HB3	1:B:311:ARG:CZ	2.23	0.69
1:B:158:LEU:HD13	1:B:167:GLN:HB3	1.75	0.68
2:C:19:DA:H2"	2:C:20:DA:C8	2.30	0.66
3:D:7:DC:H2"	3:D:8:DG:C8	2.30	0.66
1:B:141:HIS:CD2	2:C:14:DC:H41	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:DA:H8	2:C:17:DA:H5"	1.60	0.66
1:A:148:ARG:HD2	2:C:0:DT:H5"	1.78	0.65
1:B:131:LYS:NZ	3:D:2:DG:OP2	2.29	0.65
1:A:162:LEU:HB3	1:A:165:PRO:HA	1.80	0.64
1:B:28:LEU:HD12	1:B:224:ARG:HB3	1.79	0.63
1:B:79:PRO:HB3	1:B:281:TYR:CE1	2.34	0.63
1:B:40:PRO:HG3	1:B:280:PRO:HD3	1.81	0.63
1:A:133:LEU:HD23	1:A:212:ALA:HA	1.80	0.62
1:A:301:LYS:HD3	1:A:301:LYS:N	2.15	0.62
1:B:135:VAL:HA	1:B:138:THR:HG22	1.82	0.61
1:B:134:THR:HG22	1:B:137:ASP:OD2	2.00	0.61
1:A:55:GLU:OE2	1:A:332:TRP:NE1	2.31	0.60
3:D:16:DG:H2'	3:D:17:DA:C8	2.36	0.60
1:B:268:TYR:CE2	1:B:270:PRO:HB3	2.37	0.60
1:A:244:PRO:O	1:A:248:ILE:HG23	2.02	0.59
1:A:156:PRO:HG2	1:A:167:GLN:OE1	2.03	0.59
1:B:80:CYS:HB2	1:B:102:LEU:HD12	1.84	0.59
1:A:61:ASN:CG	1:A:239:LYS:HE2	2.24	0.58
1:A:40:PRO:HG3	1:A:280:PRO:HD3	1.86	0.58
1:B:163:ASN:O	1:B:165:PRO:HD3	2.03	0.58
3:D:4:DC:H2"	3:D:5:DG:C8	2.39	0.58
1:B:135:VAL:HA	1:B:138:THR:CG2	2.33	0.57
1:B:102:LEU:HB2	1:B:264:PHE:CE1	2.39	0.57
1:A:303:GLU:HB2	1:A:312:HIS:NE2	2.19	0.57
1:B:158:LEU:CD1	1:B:167:GLN:HB3	2.34	0.57
1:B:170:VAL:HG22	1:B:180:ARG:HG2	1.87	0.57
1:A:172:LYS:HA	1:A:177:ASN:O	2.03	0.57
1:B:171:ALA:HB2	1:B:223:LEU:HD23	1.86	0.56
1:B:127:ARG:HB2	1:B:217:ARG:HB3	1.86	0.56
1:A:138:THR:HG21	1:A:208:VAL:HA	1.85	0.56
1:B:106:SER:HB2	1:B:261:LYS:HE3	1.88	0.56
3:D:19:DA:H2"	3:D:20:DA:C8	2.41	0.56
1:B:217:ARG:HD2	1:B:221:GLY:HA2	1.87	0.56
1:B:29:TRP:CD2	1:B:87:LEU:HD13	2.41	0.55
3:D:1:DT:H1'	3:D:2:DG:C8	2.41	0.55
2:C:16:DG:H2'	2:C:17:DA:C8	2.42	0.55
1:A:333:ARG:NH1	1:A:350:ARG:O	2.40	0.55
3:D:3:DT:H2"	3:D:4:DC:H5'	1.88	0.55
1:A:253:ALA:HB2	1:B:248:ILE:HD11	1.87	0.55
1:A:107:GLU:N	1:A:107:GLU:OE2	2.39	0.55
1:A:228:ARG:HD3	1:A:271:ARG:NH1	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:PHE:HA	1:A:224:ARG:O	2.06	0.55
1:B:90:ASP:HB3	1:B:95:GLU:HG2	1.87	0.55
1:B:141:HIS:CD2	2:C:14:DC:N4	2.75	0.54
3:D:16:DG:H8	3:D:16:DG:H5"	1.72	0.54
1:B:159:ASP:OD2	1:B:161:SER:OG	2.23	0.54
2:C:17:DA:H5"	2:C:17:DA:C8	2.41	0.54
1:A:27:GLU:OE2	1:A:126:SER:HB2	2.07	0.54
1:A:217:ARG:HD2	1:A:221:GLY:HA2	1.89	0.54
1:B:343:SER:C	1:B:345:SER:H	2.11	0.53
1:A:104:PRO:HG2	1:A:257:ALA:O	2.08	0.53
1:B:74:LEU:HD11	1:B:255:ALA:HA	1.90	0.53
1:A:171:ALA:O	1:A:178:GLU:HA	2.09	0.53
1:A:144:PHE:HE2	1:A:146:VAL:HG22	1.74	0.53
3:D:17:DA:H2"	3:D:18:DC:O4'	2.08	0.53
2:C:0:DT:H6	2:C:0:DT:O5'	1.92	0.52
2:C:17:DA:H2"	2:C:18:DC:O4'	2.09	0.52
1:A:188:GLN:HB3	3:D:17:DA:OP2	2.10	0.52
1:A:132:THR:HG22	1:A:212:ALA:HB2	1.91	0.52
1:A:186:ARG:NH1	3:D:15:DC:OP2	2.42	0.51
1:A:248:ILE:HD11	1:B:253:ALA:HB2	1.92	0.51
1:B:284:TYR:CZ	1:B:288:VAL:HG21	2.46	0.51
2:C:15:DC:H2'	2:C:16:DG:C8	2.46	0.51
1:A:162:LEU:O	1:A:162:LEU:HD23	2.11	0.51
1:A:149:ARG:HH11	1:A:307:PRO:HG2	1.75	0.51
1:B:76:ALA:CB	1:B:330:SER:HB2	2.42	0.50
1:A:156:PRO:HG2	1:A:167:GLN:CD	2.32	0.50
2:C:2:DG:H2'	2:C:3:DT:H71	1.94	0.50
1:A:78:ILE:HG22	1:A:80:CYS:SG	2.52	0.50
1:A:288:VAL:HG22	1:A:331:GLU:HG3	1.94	0.50
1:B:134:THR:HG22	1:B:137:ASP:CG	2.32	0.50
1:A:30:TYR:HE2	1:A:38:ALA:HA	1.76	0.49
1:A:131:LYS:NZ	1:A:145:SER:O	2.46	0.49
1:B:208:VAL:HG23	1:B:209:ALA:O	2.13	0.49
1:A:283:LYS:HG2	1:A:354:TRP:HB2	1.93	0.49
2:C:3:DT:H2"	2:C:4:DC:H5'	1.95	0.49
1:A:216:LEU:O	1:A:223:LEU:HA	2.13	0.48
1:A:134:THR:HG23	1:A:137:ASP:H	1.77	0.48
1:A:60:PHE:CG	1:B:240:VAL:HG12	2.49	0.47
1:A:61:ASN:OD1	1:A:239:LYS:HE2	2.14	0.47
1:B:301:LYS:HA	1:B:311:ARG:HG2	1.96	0.47
1:A:188:GLN:OE1	1:A:189:PRO:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:PRO:O	1:B:191:ARG:HG3	2.15	0.47
1:B:268:TYR:OH	1:B:276:GLU:HG3	2.15	0.47
1:A:296:GLN:HE21	1:A:358:PRO:HB3	1.80	0.46
1:B:198:TRP:O	1:B:202:VAL:HG23	2.15	0.46
1:A:56:GLN:NE2	1:A:267:ILE:O	2.44	0.46
1:B:127:ARG:CB	1:B:217:ARG:HB3	2.46	0.46
1:B:127:ARG:CD	1:B:217:ARG:HG2	2.42	0.46
1:B:191:ARG:NH2	3:D:2:DG:N7	2.64	0.46
3:D:7:DC:C2'	3:D:8:DG:C8	2.98	0.46
1:B:255:ALA:O	1:B:259:THR:HG23	2.16	0.46
3:D:20:DA:C8	3:D:20:DA:H5"	2.51	0.46
1:B:93:SER:HA	1:B:229:ARG:HH21	1.79	0.46
1:B:217:ARG:HG3	1:B:218:GLY:O	2.15	0.46
3:D:11:DT:H2'	3:D:12:DC:C6	2.51	0.46
1:B:217:ARG:CD	1:B:221:GLY:HA2	2.46	0.45
1:B:303:GLU:O	1:B:304:SER:HB2	2.17	0.45
1:A:168:GLU:OE1	1:A:180:ARG:HD3	2.17	0.45
1:B:69:ILE:O	1:B:69:ILE:HG22	2.17	0.45
1:B:77:VAL:HG11	1:B:284:TYR:CZ	2.52	0.45
1:B:77:VAL:HG11	1:B:284:TYR:OH	2.16	0.45
1:A:30:TYR:CE2	1:A:38:ALA:HA	2.52	0.45
1:A:79:PRO:HB3	1:A:281:TYR:CE1	2.52	0.45
1:A:243:SER:HA	1:A:246:MET:HE2	1.99	0.44
1:A:298:PHE:HE2	1:A:337:VAL:HB	1.82	0.44
2:C:2:DG:H5"	2:C:2:DG:H8	1.81	0.44
1:B:179:TRP:CZ2	1:B:205:LYS:HE2	2.52	0.44
2:C:0:DT:H2"	2:C:1:DT:H5'	1.99	0.44
1:B:28:LEU:HB3	1:B:174:LEU:HD21	1.98	0.44
1:A:31:ALA:HB3	1:A:214:LEU:HD21	2.00	0.44
1:B:77:VAL:HG13	1:B:77:VAL:O	2.17	0.44
1:B:321:ASP:OD2	1:B:329:GLY:N	2.31	0.44
1:A:91:PRO:HA	1:A:175:HIS:NE2	2.33	0.44
1:B:170:VAL:HG13	1:B:180:ARG:HG3	1.98	0.43
1:A:148:ARG:HH11	2:C:0:DT:H5"	1.83	0.43
1:A:30:TYR:OH	1:A:39:LEU:HB2	2.18	0.43
1:B:283:LYS:HG2	1:B:354:TRP:HB2	1.99	0.43
1:A:243:SER:HB3	1:A:244:PRO:HD3	1.99	0.43
1:B:144:PHE:HB3	1:B:194:LEU:HB2	2.00	0.43
1:B:228:ARG:HD3	1:B:271:ARG:NH1	2.33	0.43
1:A:74:LEU:HA	1:A:74:LEU:HD12	1.58	0.43
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:GLN:OE1	1:B:309:ASP:OD2	2.36	0.43
1:A:88:SER:HB2	1:A:97:TYR:CE1	2.53	0.43
1:A:179:TRP:CZ2	1:A:205:LYS:HE2	2.52	0.43
1:B:158:LEU:HD12	1:B:159:ASP:H	1.84	0.43
1:A:45:VAL:HG12	1:A:281:TYR:HB2	2.00	0.43
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.72	0.43
1:A:134:THR:HG22	1:A:137:ASP:CG	2.39	0.43
1:A:191:ARG:NH2	2:C:2:DG:O6	2.52	0.42
1:A:197:GLY:HA2	1:A:200:VAL:HG22	2.01	0.42
1:A:208:VAL:O	1:A:211:ASP:HB2	2.19	0.42
1:A:267:ILE:HG13	1:B:242:THR:HG23	2.01	0.42
2:C:7:DC:H4'	2:C:8:DG:OP1	2.19	0.42
1:A:65:LEU:HD22	1:A:67:ALA:H	1.85	0.42
1:B:49:LEU:HD11	1:B:354:TRP:CZ2	2.54	0.42
1:B:55:GLU:OE2	1:B:332:TRP:NE1	2.44	0.42
1:A:63:GLN:O	1:A:63:GLN:HG3	2.19	0.42
1:B:30:TYR:OH	1:B:39:LEU:HB2	2.20	0.42
1:B:287:ALA:HB1	1:B:353:PRO:HB2	2.02	0.41
2:C:13:DG:H1	3:D:7:DC:H42	1.67	0.41
1:A:173:ASP:HA	1:A:225:VAL:O	2.19	0.41
1:B:243:SER:HA	1:B:246:MET:CE	2.45	0.41
1:A:134:THR:HG21	2:C:2:DG:H5'	2.03	0.41
1:B:74:LEU:HD12	1:B:74:LEU:HA	1.66	0.41
1:A:144:PHE:HB2	1:A:198:TRP:NE1	2.36	0.41
1:B:42:VAL:HG22	1:B:85:ILE:HD12	2.03	0.41
1:A:255:ALA:O	1:A:259:THR:HG23	2.20	0.41
1:B:301:LYS:HG2	1:B:301:LYS:O	2.20	0.41
1:A:122:PRO:HB2	1:A:123:LYS:H	1.60	0.41
1:A:182:ARG:HH21	1:A:184:ILE:HD12	1.86	0.41
1:B:56:GLN:O	1:B:59:SER:HB3	2.21	0.41
3:D:7:DC:H2"	3:D:8:DG:O5'	2.21	0.41
1:B:145:SER:HA	1:B:193:LEU:HD23	2.03	0.41
1:B:39:LEU:HD23	1:B:39:LEU:HA	1.88	0.40
1:A:140:THR:H	1:A:140:THR:HG23	1.60	0.40
1:B:303:GLU:H	1:B:303:GLU:HG2	1.61	0.40
1:A:133:LEU:HD23	1:A:212:ALA:CA	2.51	0.40
1:A:198:TRP:O	1:A:201:PHE:HB3	2.22	0.40
1:B:103:CYS:HB2	1:B:263:ARG:HG2	2.03	0.40
1:B:333:ARG:NH1	1:B:350:ARG:O	2.55	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	312/366 (85%)	296 (95%)	15 (5%)	1 (0%)	41 73
1	B	306/366 (84%)	281 (92%)	21 (7%)	4 (1%)	12 41
All	All	618/732 (84%)	577 (93%)	36 (6%)	5 (1%)	19 53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	343	SER
1	B	127	ARG
1	B	344	SER
1	A	310	ARG
1	B	164	PRO

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	276/316 (87%)	267 (97%)	9 (3%)	38 70
1	B	273/316 (86%)	266 (97%)	7 (3%)	46 75
All	All	549/632 (87%)	533 (97%)	16 (3%)	42 73

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU

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Mol	Chain	Res	Type
1	A	138	THR
1	A	208	VAL
1	A	219	GLU
1	A	241	LEU
1	A	263	ARG
1	A	301	LYS
1	A	309	ASP
1	A	351	VAL
1	B	126	SER
1	B	186	ARG
1	B	272	SER
1	B	282	SER
1	B	301	LYS
1	B	309	ASP
1	B	330	SER

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	167	GLN
1	B	61	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 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	318/366 (86%)	0.19	21 (6%) 18 10	51, 96, 182, 224	0
1	B	314/366 (85%)	0.34	29 (9%) 9 5	53, 99, 178, 225	0
2	C	22/22 (100%)	-0.55	0 100 100	105, 120, 235, 309	2 (9%)
3	D	22/22 (100%)	-0.80	0 100 100	85, 139, 191, 193	2 (9%)
All	All	676/776 (87%)	0.20	50 (7%) 14 8	51, 99, 191, 309	4 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	GLN	7.7
1	B	304	SER	6.0
1	B	302	PHE	5.4
1	B	61	ASN	5.4
1	B	236	LEU	5.2
1	B	307	PRO	5.2
1	B	36	GLN	4.8
1	A	307	PRO	4.7
1	A	304	SER	4.5
1	A	62	ASN	4.5
1	B	347	ARG	4.3
1	A	303	GLU	4.3
1	B	24	ILE	3.9
1	A	60	PHE	3.8
1	A	305	GLU	3.8
1	A	346	GLU	3.8
1	A	302	PHE	3.8
1	B	345	SER	3.7
1	A	343	SER	3.7
1	B	238	PRO	3.4
1	B	310	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	219	GLU	3.3
1	B	303	GLU	3.3
1	B	346	GLU	3.2
1	B	348	GLN	3.2
1	B	361	SER	3.2
1	B	344	SER	2.9
1	A	68	GLN	2.9
1	A	345	SER	2.8
1	B	298	PHE	2.7
1	B	234	GLN	2.7
1	B	300	MET	2.6
1	B	108	GLN	2.6
1	A	159	ASP	2.5
1	B	60	PHE	2.5
1	B	217	ARG	2.5
1	A	61	ASN	2.5
1	B	235	GLN	2.5
1	A	64	GLU	2.4
1	B	174	LEU	2.4
1	A	94	ASP	2.4
1	A	153	ASP	2.3
1	B	178	GLU	2.3
1	A	310	ARG	2.2
1	A	194	LEU	2.2
1	A	311	ARG	2.2
1	B	216	LEU	2.2
1	A	341	GLU	2.2
1	B	69	ILE	2.1
1	B	72	TYR	2.1

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.