Full wwPDB X-ray Structure Validation Report (i)

Mar 13, 2024 – 03:46 PM JST

PDB ID	:	5AWH
Title	:	Rhodobacter sphaeroides Argonaute in complex with guide RNA/target DNA heteroduplex
Authors	:	Miyoshi, T.; Ito, K.; Murakami, R.; Uchiumi, T.
Deposited on	:	2015-07-03
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 (i) 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 (1)) were used in the production of this report:

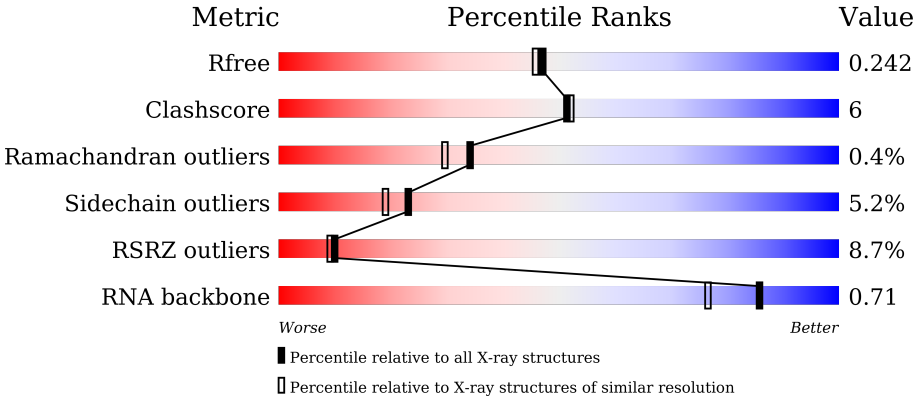
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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)
RNA backbone	3102	1079 (2.50-1.50)

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	778	6% 81% 14% • •
1	B	778	11% 81% 10% • 8%
2	C	18	44% 56%
2	E	18	67% 22% 6% 6%

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Mol	Chain	Length	Quality of chain
3	D	18	6% 83% 17%
3	F	18	6% 78% 17% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13805 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	759	6005	3808	1084	1096	17	0	0	0
1	B	715	5664	3600	1027	1022	15	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP A4WYU7
A	1	GLY	-	expression tag	UNP A4WYU7
A	2	SER	-	expression tag	UNP A4WYU7
A	3	SER	-	expression tag	UNP A4WYU7
A	4	HIS	-	expression tag	UNP A4WYU7
A	5	HIS	-	expression tag	UNP A4WYU7
A	6	HIS	-	expression tag	UNP A4WYU7
A	7	HIS	-	expression tag	UNP A4WYU7
A	8	HIS	-	expression tag	UNP A4WYU7
A	9	HIS	-	expression tag	UNP A4WYU7
A	10	SER	-	expression tag	UNP A4WYU7
A	11	SER	-	expression tag	UNP A4WYU7
A	12	GLY	-	expression tag	UNP A4WYU7
A	13	LEU	-	expression tag	UNP A4WYU7
A	14	VAL	-	expression tag	UNP A4WYU7
A	15	PRO	-	expression tag	UNP A4WYU7
A	16	ALA	-	expression tag	UNP A4WYU7
A	17	GLY	-	expression tag	UNP A4WYU7
A	18	SER	-	expression tag	UNP A4WYU7
A	19	HIS	-	expression tag	UNP A4WYU7
A	20	MET	-	expression tag	UNP A4WYU7
B	0	MET	-	expression tag	UNP A4WYU7
B	1	GLY	-	expression tag	UNP A4WYU7
B	2	SER	-	expression tag	UNP A4WYU7
B	3	SER	-	expression tag	UNP A4WYU7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	HIS	-	expression tag	UNP A4WYU7
B	5	HIS	-	expression tag	UNP A4WYU7
B	6	HIS	-	expression tag	UNP A4WYU7
B	7	HIS	-	expression tag	UNP A4WYU7
B	8	HIS	-	expression tag	UNP A4WYU7
B	9	HIS	-	expression tag	UNP A4WYU7
B	10	SER	-	expression tag	UNP A4WYU7
B	11	SER	-	expression tag	UNP A4WYU7
B	12	GLY	-	expression tag	UNP A4WYU7
B	13	LEU	-	expression tag	UNP A4WYU7
B	14	VAL	-	expression tag	UNP A4WYU7
B	15	PRO	-	expression tag	UNP A4WYU7
B	16	ALA	-	expression tag	UNP A4WYU7
B	17	GLY	-	expression tag	UNP A4WYU7
B	18	SER	-	expression tag	UNP A4WYU7
B	19	HIS	-	expression tag	UNP A4WYU7
B	20	MET	-	expression tag	UNP A4WYU7

- Molecule 2 is a RNA chain called RNA (5'-D(P*UP*UP*AP*CP*AP*AP*CP*CP*UP*AP*CP*UP*AP*CP*CP*UP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	18	374	168	61	127	18	0	0	0
2	E	18	374	168	61	127	18	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(*CP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*GP*TP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	18	375	179	73	106	17	0	0	0
3	F	18	375	179	73	106	17	0	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	C	1	1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	E	1	1	1	0	0

- Molecule 5 is water.

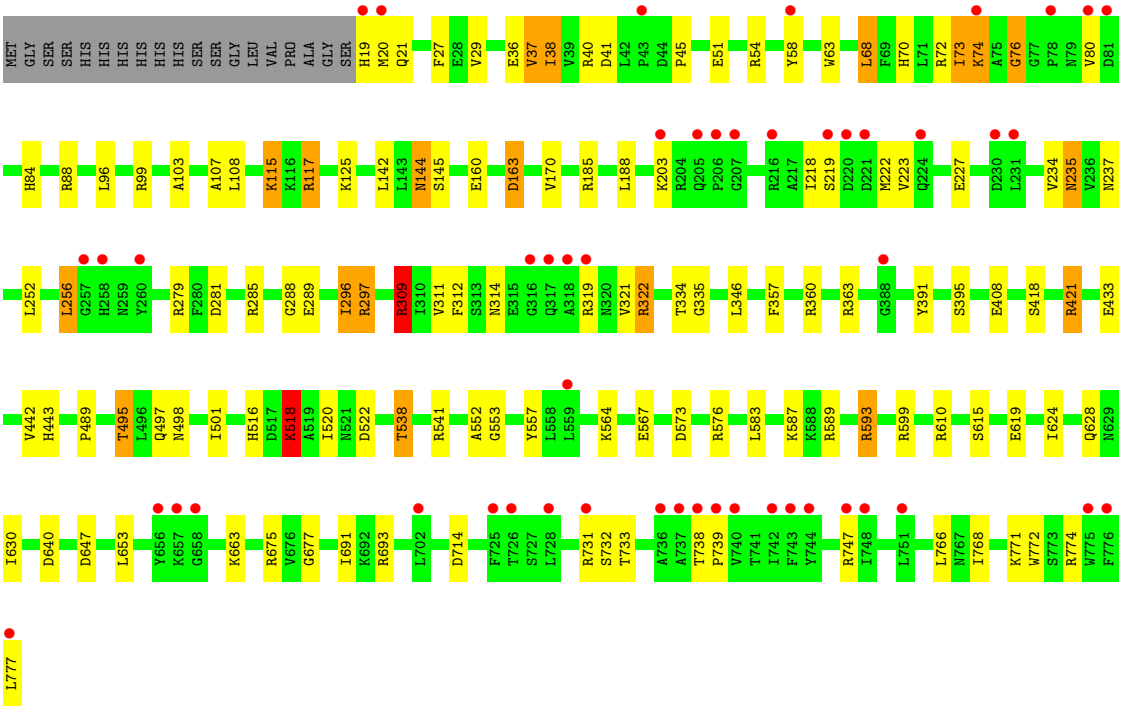
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	292	292	292	0	0
			Total	O		
5	B	182	182	182	0	0
			Total	O		
5	C	50	50	50	0	0
			Total	O		
5	D	57	57	57	0	0
			Total	O		
5	E	30	30	30	0	0
			Total	O		
5	F	25	25	25	0	0

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.

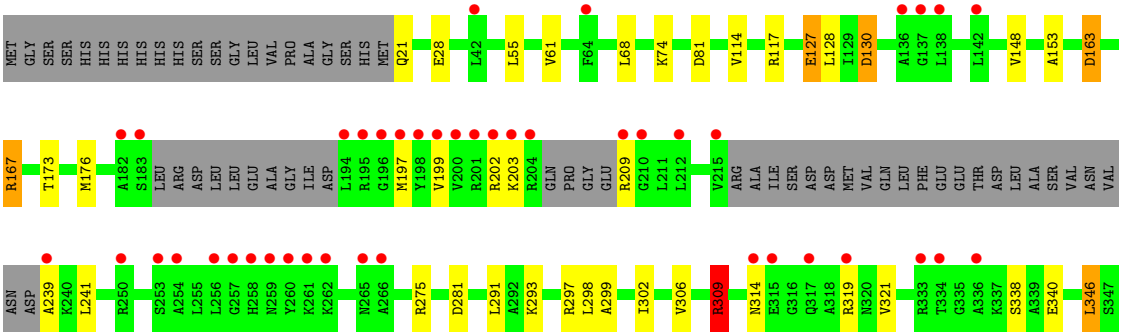
- Molecule 1: Uncharacterized protein

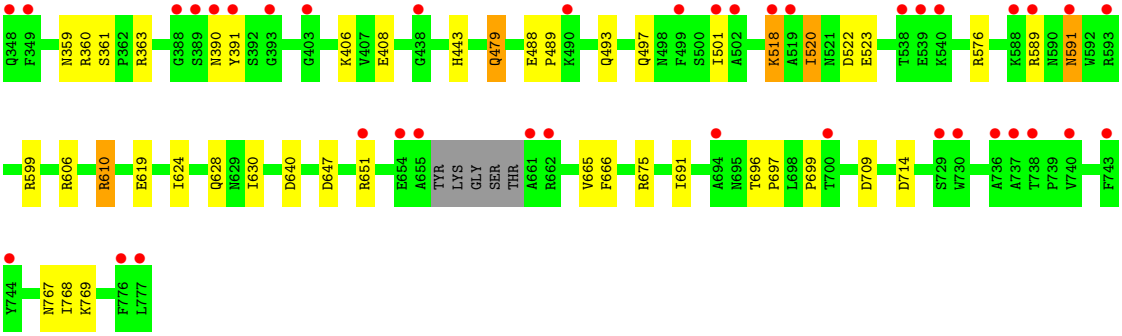
Chain A:



- Molecule 1: Uncharacterized protein

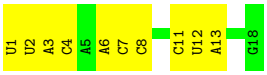
Chain B:





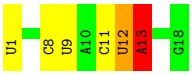
• Molecule 2: RNA (5'-D(P*UP*UP*AP*CP*AP*AP*CP*CP*UP*AP*CP*UP*AP*CP*CP*UP*CP*G)-3')

Chain C:



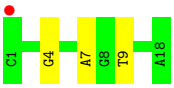
• Molecule 2: RNA (5'-D(P*UP*UP*AP*CP*AP*AP*CP*CP*UP*AP*CP*UP*AP*CP*CP*UP*CP*G)-3')

Chain E:



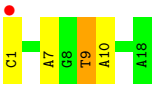
• Molecule 3: DNA (5'-D(*CP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*GP*TP*AP*A)-3')

Chain D:



• Molecule 3: DNA (5'-D(*CP*GP*AP*GP*GP*TP*AP*GP*TP*AP*GP*GP*TP*TP*GP*TP*AP*A)-3')

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.19Å 118.30Å 118.48Å 90.00° 95.83° 90.00°	Depositor
Resolution (Å)	35.63 – 2.00 35.60 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.1 (35.63-2.00) 97.1 (35.60-1.99)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.56 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.184 , 0.233 0.194 , 0.242	Depositor DCC
R_{free} test set	6232 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 65.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13805	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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 (i)

5.1 Standard geometry (i)

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

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	0.89	2/6136 (0.0%)	0.95	14/8305 (0.2%)
1	B	0.75	0/5787	0.89	9/7826 (0.1%)
2	C	0.98	1/415 (0.2%)	1.02	1/640 (0.2%)
2	E	0.88	1/415 (0.2%)	1.03	2/640 (0.3%)
3	D	0.80	1/422 (0.2%)	1.00	1/652 (0.2%)
3	F	0.62	0/422	0.94	1/652 (0.2%)
All	All	0.82	5/13597 (0.0%)	0.93	28/18715 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	U	OP3-P	-11.11	1.47	1.61
2	C	1	U	OP3-P	-7.72	1.51	1.61
1	A	615	SER	CB-OG	-7.14	1.32	1.42
3	D	9	DT	O3'-P	-5.79	1.54	1.61
1	A	567	GLU	CG-CD	5.56	1.60	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	13	A	O5'-P-OP2	-11.31	95.52	105.70
1	B	610	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	B	610	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	599	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	567	GLU	OE1-CD-OE2	-7.36	114.46	123.30
3	F	9	DT	O5'-P-OP2	-6.90	99.49	105.70
1	A	117	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	B	309	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	B	309	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	167	ARG	NE-CZ-NH1	6.09	123.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	714	ASP	CB-CG-OD1	6.05	123.74	118.30
2	C	8	C	O5'-P-OP2	-5.93	100.36	105.70
1	A	599	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	573	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	541	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	163	ASP	CB-CG-OD1	5.64	123.37	118.30
1	A	309	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	88	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	309	ARG	CG-CD-NE	-5.57	100.11	111.80
1	B	81	ASP	CB-CG-OD1	5.52	123.27	118.30
3	D	4	DG	C1'-O4'-C4'	-5.43	104.67	110.10
1	B	346	LEU	CB-CG-CD2	5.34	120.08	111.00
2	E	13	A	O5'-P-OP1	5.28	117.03	110.70
1	B	360	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	99	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	115	LYS	CD-CE-NZ	5.10	123.44	111.70
1	A	99	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	693	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	6005	0	6039	83	0
1	B	5664	0	5713	53	0
2	C	374	0	194	5	0
2	E	374	0	194	3	0
3	D	375	0	205	1	0
3	F	375	0	205	3	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	292	0	0	9	0
5	B	182	0	0	4	0
5	C	50	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	57	0	0	0	0
5	E	30	0	0	0	0
5	F	25	0	0	0	0
All	All	13805	0	12550	144	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 6.

All (144) 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:148:VAL:HG12	1:B:176:MET:CE	1.99	0.93
1:B:606:ARG:HG2	5:B:966:HOH:O	1.78	0.84
1:B:363:ARG:H	1:B:443:HIS:HD2	1.24	0.83
1:B:363:ARG:H	1:B:443:HIS:CD2	1.99	0.80
1:A:610:ARG:CZ	5:A:802:HOH:O	2.33	0.77
1:A:227:GLU:O	1:A:538:THR:HG21	1.86	0.75
1:A:363:ARG:H	1:A:443:HIS:HD2	1.31	0.74
1:B:148:VAL:HG12	1:B:176:MET:HE2	1.69	0.73
1:A:610:ARG:NH2	5:A:802:HOH:O	2.23	0.71
1:A:29:VAL:CG2	1:A:170:VAL:HG23	2.21	0.70
1:A:418:SER:O	1:A:421:ARG:NH1	2.24	0.70
1:A:663:LYS:HE3	1:A:691:ILE:O	1.92	0.70
1:B:61:VAL:CG1	1:B:68:LEU:HD11	2.22	0.69
1:B:128:LEU:HD22	1:B:176:MET:CE	2.23	0.68
1:B:163:ASP:OD1	1:B:675:ARG:NH2	2.29	0.65
1:B:576:ARG:HD2	1:B:619:GLU:HG3	1.79	0.65
1:A:624:ILE:CD1	1:A:630:ILE:HD12	2.27	0.64
1:B:610:ARG:HD2	1:B:709:ASP:OD2	1.99	0.62
1:B:275:ARG:HB3	1:B:697:PRO:HB3	1.81	0.61
1:B:497:GLN:O	1:B:501:ILE:HG12	2.00	0.61
1:A:346:LEU:CD2	1:A:501:ILE:HD11	2.31	0.61
1:B:314:ASN:HD22	1:B:319:ARG:HA	1.66	0.61
1:A:576:ARG:HD2	1:A:619:GLU:HG3	1.82	0.61
1:B:128:LEU:HD22	1:B:176:MET:HE1	1.83	0.60
1:A:610:ARG:NE	5:A:802:HOH:O	2.33	0.60
1:A:58:TYR:CE1	1:A:76:GLY:O	2.54	0.60
1:B:148:VAL:HG12	1:B:176:MET:HE3	1.83	0.60
1:B:117:ARG:NH1	5:B:802:HOH:O	2.33	0.59
1:B:148:VAL:CG1	1:B:176:MET:HE2	2.32	0.59
1:A:663:LYS:CE	1:A:691:ILE:O	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ARG:NH1	1:A:289:GLU:OE2	2.36	0.58
1:B:281:ASP:OD1	1:B:309:ARG:NH2	2.36	0.58
1:A:103:ALA:HB1	1:A:296:ILE:CD1	2.33	0.58
1:A:281:ASP:OD1	1:A:309:ARG:NH2	2.34	0.58
1:A:68:LEU:HD13	1:A:70:HIS:NE2	2.19	0.58
1:B:406:LYS:HB2	5:B:855:HOH:O	2.04	0.57
1:A:296:ILE:C	1:A:296:ILE:HD12	2.26	0.56
1:A:360:ARG:HB2	5:A:1039:HOH:O	2.05	0.56
1:A:73:ILE:HD13	1:A:73:ILE:C	2.25	0.56
1:A:433:GLU:OE1	1:B:767:ASN:ND2	2.38	0.56
3:F:1:DC:H2'	3:F:1:DC:O2	2.06	0.55
1:A:640:ASP:O	3:D:7:DA:H3'	2.06	0.55
1:A:346:LEU:HD22	1:A:501:ILE:HD11	1.89	0.55
1:B:691:ILE:HD11	1:B:699:PRO:HG3	1.89	0.54
1:A:495:THR:HB	2:C:2:U:C2	2.42	0.53
1:B:148:VAL:CG1	1:B:176:MET:CE	2.80	0.53
1:A:363:ARG:H	1:A:443:HIS:CD2	2.20	0.52
1:A:223:VAL:CG1	1:A:234:VAL:HG13	2.39	0.52
1:A:237:ASN:ND2	5:A:804:HOH:O	2.34	0.52
1:A:314:ASN:HD21	1:A:321:VAL:H	1.56	0.52
1:B:127:GLU:OE1	1:B:130:ASP:OD1	2.27	0.52
1:A:29:VAL:HG21	1:A:170:VAL:HG23	1.92	0.51
1:A:252:LEU:O	1:A:256:LEU:HB2	2.10	0.51
1:A:497:GLN:O	1:A:501:ILE:HG12	2.11	0.51
1:A:589:ARG:HB2	5:A:992:HOH:O	2.11	0.51
1:A:296:ILE:HD12	1:A:297:ARG:N	2.26	0.51
1:A:731:ARG:HD2	1:A:777:LEU:OXT	2.10	0.50
2:C:12:U:H2'	2:C:13:A:O4'	2.11	0.50
1:B:299:ALA:HB3	1:B:302:ILE:HB	1.93	0.50
1:A:587:LYS:NZ	1:A:628:GLN:HE22	2.10	0.50
1:A:363:ARG:HG2	1:A:408:GLU:OE1	2.12	0.50
1:B:488:GLU:N	1:B:488:GLU:OE2	2.44	0.50
1:A:51:GLU:OE1	1:A:54:ARG:NH1	2.45	0.49
1:A:518:LYS:HD3	1:A:518:LYS:H	1.77	0.49
1:A:774:ARG:N	1:A:774:ARG:HD3	2.27	0.49
1:A:160:GLU:HB2	1:A:677:GLY:HA2	1.93	0.49
1:A:235:ASN:OD1	1:A:235:ASN:N	2.41	0.49
1:B:363:ARG:NH1	1:B:408:GLU:OE2	2.46	0.49
1:A:19:HIS:CE1	1:A:647:ASP:OD2	2.66	0.48
1:A:321:VAL:HG12	1:A:322:ARG:N	2.28	0.48
2:E:12:U:H2'	2:E:13:A:O4'	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:VAL:HG13	1:A:234:VAL:HG13	1.96	0.48
1:B:197:MET:HE3	1:B:241:LEU:HD22	1.95	0.48
2:E:8:C:H2'	2:E:9:U:C6	2.48	0.48
1:B:640:ASP:O	3:F:7:DA:H3'	2.13	0.47
2:C:3:A:H2'	2:C:4:C:C6	2.49	0.47
1:A:103:ALA:HB1	1:A:296:ILE:HD11	1.96	0.47
1:A:218:ILE:CD1	1:A:223:VAL:HB	2.45	0.47
1:A:498:ASN:ND2	1:A:733:THR:H	2.12	0.47
1:B:520:ILE:CD1	1:B:523:GLU:HB2	2.45	0.47
1:B:128:LEU:HD13	1:B:176:MET:HE1	1.97	0.46
1:B:520:ILE:HG12	1:B:599:ARG:CZ	2.44	0.46
1:A:84:HIS:ND1	5:A:807:HOH:O	2.36	0.46
1:B:691:ILE:HG23	1:B:696:THR:HG21	1.98	0.46
1:B:361:SER:HA	1:B:406:LYS:O	2.16	0.46
1:B:520:ILE:HD13	1:B:523:GLU:HB2	1.98	0.46
1:A:516:HIS:HB3	1:A:557:TYR:CE2	2.51	0.46
1:A:21:GLN:CG	1:A:311:VAL:HG11	2.47	0.45
1:A:144:ASN:HD22	1:A:144:ASN:N	2.14	0.45
1:A:334:THR:OG1	1:A:335:GLY:N	2.49	0.45
1:B:28:GLU:HB3	1:B:167:ARG:NH2	2.31	0.45
1:A:516:HIS:CE1	1:A:552:ALA:HB1	2.51	0.45
1:A:312:PHE:HB3	1:A:321:VAL:CG2	2.47	0.45
1:A:96:LEU:HD23	1:A:96:LEU:HA	1.84	0.45
1:B:651:ARG:O	1:B:651:ARG:CG	2.65	0.45
1:A:107:ALA:C	1:A:108:LEU:HD12	2.37	0.44
1:A:516:HIS:HE1	1:A:553:GLY:H	1.66	0.44
2:C:6:A:H2'	2:C:7:C:O4'	2.18	0.44
2:E:11:C:H2'	2:E:12:U:O4'	2.18	0.44
3:F:9:DT:H2"	3:F:10:DA:H5'	1.98	0.44
1:A:73:ILE:HD13	1:A:74:LYS:HB3	1.98	0.44
1:A:314:ASN:HD22	1:A:319:ARG:HA	1.82	0.44
1:B:391:TYR:CE2	1:B:489:PRO:HB2	2.52	0.44
1:A:223:VAL:HG13	1:A:234:VAL:CG1	2.47	0.44
1:A:142:LEU:O	1:A:145:SER:OG	2.26	0.44
1:A:498:ASN:ND2	1:A:732:SER:HA	2.33	0.43
1:A:593:ARG:HH11	1:A:593:ARG:CG	2.31	0.43
1:B:624:ILE:CD1	1:B:630:ILE:HD13	2.48	0.43
1:A:45:PRO:HG3	1:A:63:TRP:CZ2	2.53	0.43
1:A:346:LEU:CD2	1:A:501:ILE:CD1	2.97	0.43
1:A:117:ARG:HD3	5:A:839:HOH:O	2.18	0.43
1:A:218:ILE:HD13	1:A:223:VAL:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLN:HG3	1:A:311:VAL:HG11	2.00	0.43
2:C:11:C:H2'	2:C:12:U:O4'	2.19	0.43
1:A:73:ILE:HD13	1:A:73:ILE:O	2.19	0.43
1:A:38:ILE:HG21	1:A:80:VAL:HG23	2.00	0.42
1:B:128:LEU:HD22	1:B:176:MET:HE2	1.98	0.42
1:B:363:ARG:N	1:B:443:HIS:HD2	2.04	0.42
1:A:583:LEU:HD13	1:A:624:ILE:HD11	2.02	0.42
1:A:346:LEU:HD22	1:A:501:ILE:CD1	2.48	0.42
1:A:357:PHE:O	1:A:360:ARG:CZ	2.67	0.42
1:A:107:ALA:O	1:A:108:LEU:HD12	2.20	0.42
1:B:391:TYR:HB3	1:B:493:GLN:OE1	2.19	0.42
1:B:630:ILE:HG22	5:B:941:HOH:O	2.20	0.42
1:B:61:VAL:HG12	1:B:68:LEU:HD11	1.98	0.42
1:B:479:GLN:HE21	1:B:479:GLN:HB3	1.70	0.42
1:B:591:ASN:OD1	1:B:591:ASN:N	2.53	0.42
1:A:576:ARG:NH1	5:A:823:HOH:O	2.52	0.41
1:B:520:ILE:HD11	1:B:599:ARG:NH2	2.35	0.41
1:B:153:ALA:HB3	1:B:173:THR:OG1	2.21	0.41
1:B:714:ASP:OD1	1:B:714:ASP:C	2.59	0.41
1:A:593:ARG:HH11	1:A:593:ARG:HG3	1.86	0.41
1:B:665:VAL:O	1:B:666:PHE:HB2	2.20	0.41
1:A:312:PHE:O	1:A:321:VAL:HG21	2.20	0.41
1:A:163:ASP:OD1	1:A:675:ARG:NH1	2.49	0.41
1:A:738:THR:OG1	1:A:739:PRO:HD2	2.21	0.40
1:A:771:LYS:HE3	1:A:772:TRP:CZ2	2.56	0.40
1:B:624:ILE:CG2	1:B:628:GLN:HB2	2.50	0.40
1:B:647:ASP:O	1:B:666:PHE:HA	2.22	0.40
1:A:37:VAL:CG1	1:A:38:ILE:N	2.83	0.40
1:A:391:TYR:CE1	1:A:489:PRO:HB2	2.56	0.40
1:B:202:ARG:HG3	1:B:239:ALA:N	2.36	0.40
1:A:27:PHE:CZ	1:A:288:GLY:HA3	2.57	0.40
1:B:314:ASN:HD21	1:B:321:VAL:H	1.69	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	757/778 (97%)	728 (96%)	25 (3%)	4 (0%)	29	23
1	B	705/778 (91%)	686 (97%)	17 (2%)	2 (0%)	41	37
All	All	1462/1556 (94%)	1414 (97%)	42 (3%)	6 (0%)	34	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	518	LYS
1	A	76	GLY
1	A	518	LYS
1	A	522	ASP
1	B	768	ILE
1	A	768	ILE

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	643/658 (98%)	605 (94%)	38 (6%)	19	15
1	B	605/658 (92%)	578 (96%)	27 (4%)	27	24
All	All	1248/1316 (95%)	1183 (95%)	65 (5%)	23	19

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	MET
1	A	36	GLU
1	A	37	VAL
1	A	38	ILE
1	A	40	ARG
1	A	41	ASP

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Mol	Chain	Res	Type
1	A	68	LEU
1	A	72	ARG
1	A	73	ILE
1	A	74	LYS
1	A	115	LYS
1	A	125	LYS
1	A	144	ASN
1	A	163	ASP
1	A	185	ARG
1	A	188	LEU
1	A	203	LYS
1	A	219	SER
1	A	222	MET
1	A	235	ASN
1	A	256	LEU
1	A	279	ARG
1	A	296	ILE
1	A	297	ARG
1	A	309	ARG
1	A	322	ARG
1	A	395	SER
1	A	421	ARG
1	A	442	VAL
1	A	495	THR
1	A	518	LYS
1	A	520	ILE
1	A	538	THR
1	A	564	LYS
1	A	593	ARG
1	A	653	LEU
1	A	747	ARG
1	A	766	LEU
1	B	21	GLN
1	B	55	LEU
1	B	74	LYS
1	B	114	VAL
1	B	127	GLU
1	B	130	ASP
1	B	199	VAL
1	B	203	LYS
1	B	209	ARG
1	B	291	LEU

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Mol	Chain	Res	Type
1	B	293	LYS
1	B	297	ARG
1	B	298	LEU
1	B	306	VAL
1	B	309	ARG
1	B	338	SER
1	B	340	GLU
1	B	346	LEU
1	B	359	ASN
1	B	390	ASN
1	B	479	GLN
1	B	518	LYS
1	B	520	ILE
1	B	522	ASP
1	B	589	ARG
1	B	591	ASN
1	B	769	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	124	GLN
1	A	144	ASN
1	A	259	ASN
1	A	303	ASN
1	A	314	ASN
1	A	422	ASN
1	A	443	HIS
1	A	479	GLN
1	A	498	ASN
1	A	516	HIS
1	A	628	GLN
1	B	314	ASN
1	B	422	ASN
1	B	443	HIS
1	B	465	HIS
1	B	479	GLN
1	B	508	ASN
1	B	590	ASN
1	B	689	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	17/18 (94%)	0	0
2	E	17/18 (94%)	2 (11%)	0
All	All	34/36 (94%)	2 (5%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	12	U
2	E	13	A

There are no RNA pucker outliers to report.

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	759/778 (97%)	0.17	50 (6%) 18 17	29, 51, 85, 110	0
1	B	715/778 (91%)	0.50	82 (11%) 4 4	34, 62, 99, 130	0
2	C	18/18 (100%)	-0.80	0 100 100	34, 41, 62, 80	0
2	E	18/18 (100%)	-0.72	0 100 100	43, 53, 70, 86	0
3	D	18/18 (100%)	-0.39	1 (5%) 24 23	39, 47, 74, 99	0
3	F	18/18 (100%)	-0.28	1 (5%) 24 23	41, 64, 74, 106	0
All	All	1546/1628 (94%)	0.29	134 (8%) 10 9	29, 56, 92, 130	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	389	SER	7.0
1	B	196	GLY	6.9
1	B	215	VAL	6.7
1	A	317	GLN	6.7
1	B	204	ARG	6.5
1	B	519	ALA	6.4
1	B	260	TYR	6.4
1	B	388	GLY	6.3
1	B	258	HIS	5.9
1	A	258	HIS	5.8
1	B	262	LYS	5.5
1	B	317	GLN	5.5
1	B	253	SER	5.0
1	A	58	TYR	4.9
1	B	209	ARG	4.9
1	B	694	ALA	4.8
1	B	256	LEU	4.8
1	B	210	GLY	4.6
1	B	183	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	239	ALA	4.3
1	B	194	LEU	4.2
1	A	206	PRO	4.2
1	B	390	ASN	4.2
1	A	744	TYR	3.9
1	A	205	GLN	3.8
1	B	254	ALA	3.8
1	A	656	TYR	3.7
1	B	201	ARG	3.7
1	B	589	ARG	3.6
1	B	257	GLY	3.6
1	B	336	ALA	3.6
1	B	661	ALA	3.6
1	B	212	LEU	3.6
1	A	43	PRO	3.6
1	B	334	THR	3.5
1	B	591	ASN	3.5
1	A	207	GLY	3.5
1	B	349	PHE	3.4
1	B	391	TYR	3.3
1	A	737	ALA	3.3
1	B	259	ASN	3.3
1	A	19	HIS	3.3
1	B	333	ARG	3.2
1	A	318	ALA	3.2
1	A	775	TRP	3.2
1	B	137	GLY	3.2
1	B	195	ARG	3.2
1	A	657	LYS	3.1
1	A	776	PHE	3.0
1	A	78	PRO	3.0
1	B	490	LYS	3.0
3	F	1	DC	3.0
1	A	221	ASP	3.0
1	A	231	LEU	3.0
1	B	261	LYS	2.9
3	D	1	DC	2.9
1	B	662	ARG	2.9
1	A	260	TYR	2.9
1	B	593	ARG	2.9
1	B	655	ALA	2.9
1	B	203	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	81	ASP	2.9
1	A	658	GLY	2.9
1	A	743	PHE	2.9
1	A	216	ARG	2.9
1	A	220	ASP	2.8
1	A	738	THR	2.8
1	B	314	ASN	2.8
1	A	219	SER	2.8
1	B	199	VAL	2.7
1	B	200	VAL	2.7
1	B	738	THR	2.7
1	B	182	ALA	2.7
1	B	438	GLY	2.6
1	A	80	VAL	2.6
1	A	230	ASP	2.6
1	B	777	LEU	2.6
1	B	744	TYR	2.5
1	A	316	GLY	2.5
1	A	319	ARG	2.5
1	B	198	TYR	2.5
1	A	736	ALA	2.5
1	B	743	PHE	2.5
1	A	740	VAL	2.4
1	A	20	MET	2.4
1	B	740	VAL	2.4
1	B	518	LYS	2.4
1	B	265	ASN	2.4
1	B	737	ALA	2.4
1	A	559	LEU	2.4
1	B	588	LYS	2.3
1	B	319	ARG	2.3
1	B	539	GLU	2.3
1	A	702	LEU	2.3
1	A	777	LEU	2.3
1	B	42	LEU	2.3
1	B	197	MET	2.3
1	B	729	SER	2.3
1	B	654	GLU	2.3
1	A	731	ARG	2.2
1	A	748	ILE	2.2
1	B	136	ALA	2.2
1	B	700	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	257	GLY	2.2
1	B	403	GLY	2.2
1	B	499	PHE	2.2
1	A	739	PRO	2.2
1	B	538	THR	2.2
1	B	730	TRP	2.2
1	B	138	LEU	2.2
1	B	266	ALA	2.2
1	B	736	ALA	2.2
1	A	203	LYS	2.2
1	A	224	GLN	2.1
1	A	747	ARG	2.2
1	B	250	ARG	2.1
1	B	348	GLN	2.1
1	B	502	ALA	2.1
1	A	751	LEU	2.1
1	B	540	LYS	2.1
1	B	202	ARG	2.1
1	B	64	PHE	2.1
1	B	142	LEU	2.1
1	B	776	PHE	2.1
1	B	651	ARG	2.1
1	B	393	GLY	2.1
1	B	315	GLU	2.1
1	A	74	LYS	2.1
1	A	725	PHE	2.0
1	A	388	GLY	2.0
1	B	501	ILE	2.0
1	A	726	THR	2.0
1	A	728	LEU	2.0
1	A	742	ILE	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, 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(Å^2)	Q<0.9
4	MG	C	101	1/1	0.98	0.15	33,33,33,33	0
4	MG	E	101	1/1	0.98	0.16	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.