Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:28 PM GMT

PDB ID : 4P0P
Title : Crystal structure of Human Mus81-Eme1 in complex with 5'-flap DNA, and Mg2+
Authors : Gwon, G.H.; Baek, K.; Cho, Y.
Deposited on : 2014-02-22
Resolution : 2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

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 2.80 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	Percentile Ranks	Value
Rfree		0.246
Clashscore		10
Ramachandran outliers		0.5%
Sidechain outliers		6.2%
RSRZ outliers		8.1%

Worse 　　　　　*Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
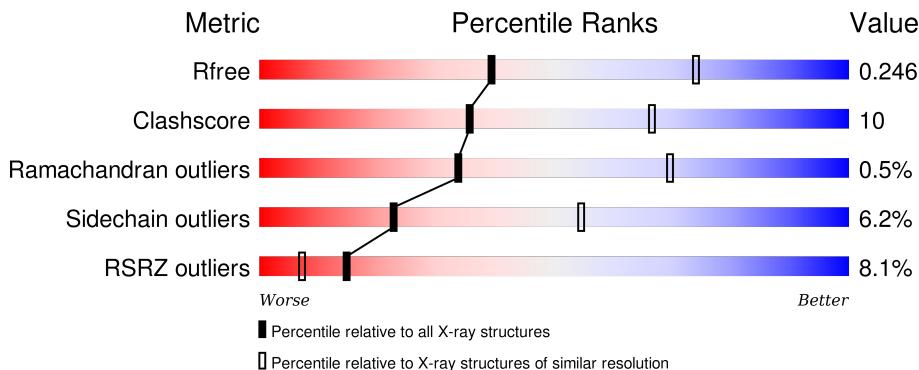
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	306	5% / 79% / 12% · 8%
2	B	393	6% / 58% / 12% · 29%
3	E	17	29% / 41% / 53% / 6%
4	F	6	33% / 33% / 67%
5	G	16	13% / 38% / 25% / 6% / 31%
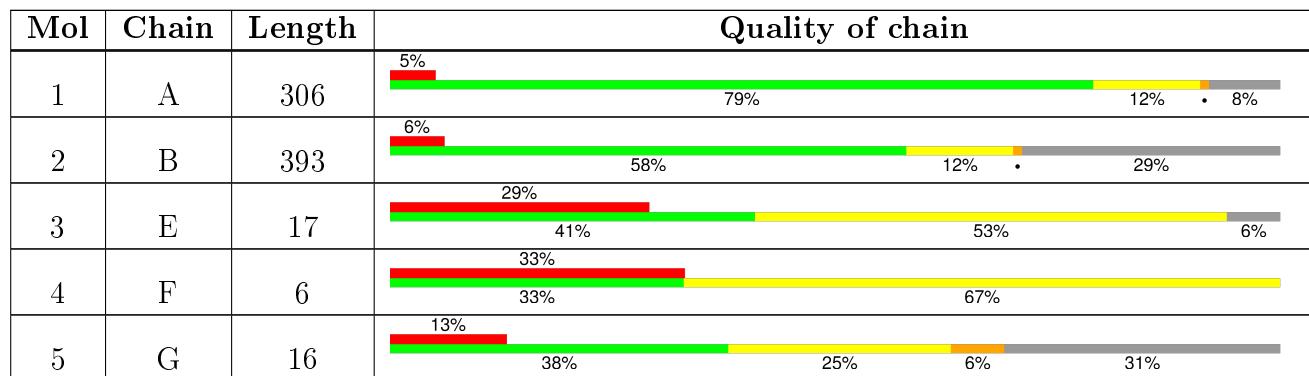
2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5147 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 Crossover junction endonuclease MUS81.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2234	1402	415	409	8			

- Molecule 2 is a protein called Crossover junction endonuclease EME1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	278	Total	C	N	O	S	0	0	0
			2187	1376	390	407	14			

- Molecule 3 is a DNA chain called DNA GAATGTGTGTCTCAATC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	16	Total	C	N	O	P	0	0	0
			327	157	56	98	16			

- Molecule 4 is a DNA chain called DNA GGATTG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	6	Total	C	N	O	P	0	0	0
			127	60	24	37	6			

- Molecule 5 is a DNA chain called DNA TAACCAGACACACATT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	11	Total	C	N	O	P	0	0	0
			224	107	43	63	11			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

• Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	21	Total 21	O 21	0	0
7	B	18	Total 18	O 18	0	0
7	E	4	Total 4	O 4	0	0
7	F	1	Total 1	O 1	0	0
7	G	3	Total 3	O 3	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Crossover junction endonuclease MUS81
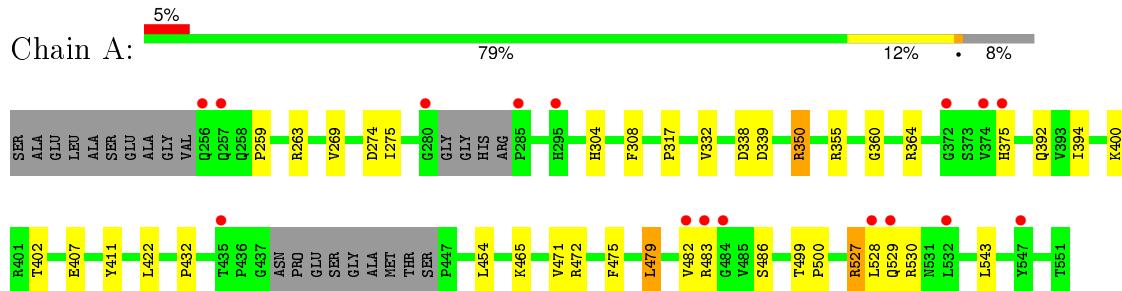
- Molecule 2: Crossover junction endonuclease EME1
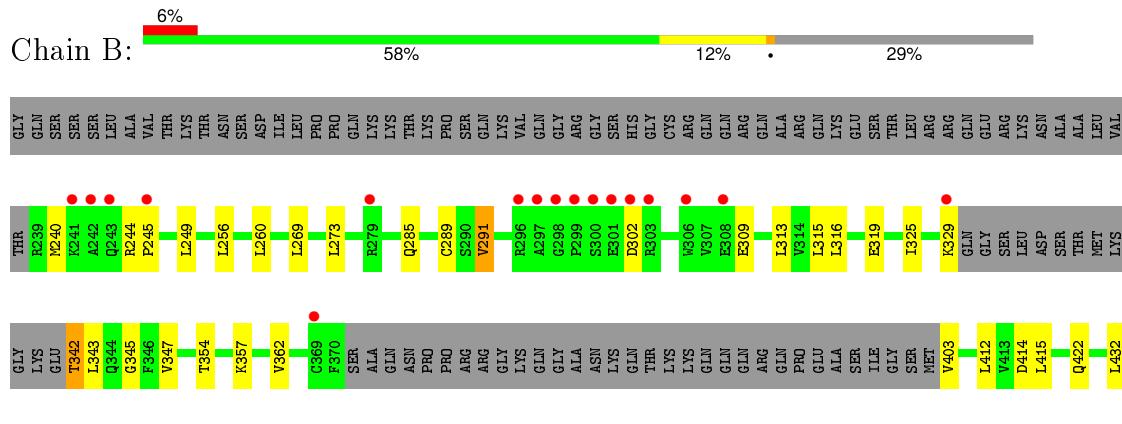
- Molecule 3: DNA GAATGTGTGTCTCAATC
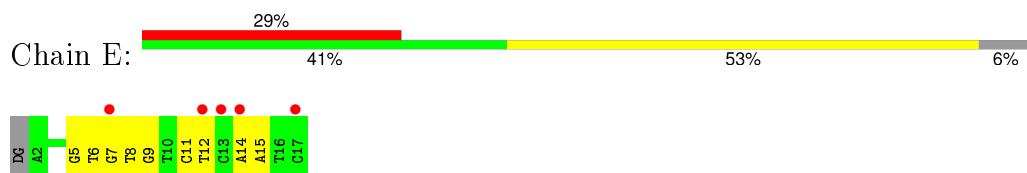
- Molecule 4: DNA GGATTG

G21 G22 A23 T24 T25 G26

● Molecule 5: DNA TAACCAGACACACATT

Chain G:

13%

38%   25%   6%   31%

DT DA DA DC DC A28 G29 A30 C31 A32 C33 A34 C35 A36 T37 T38

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	85.02Å 226.50Å 52.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.03 – 2.80 47.60 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.8 (33.03-2.80) 95.2 (47.60-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.222 , 0.243 0.224 , 0.246	Depositor DCC
R_{free} test set	1265 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	78.2	Xtriage
Anisotropy	0.429	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Outliers	0 of 27024 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5147	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.22	0/2273	0.40	0/3073
2	B	0.22	0/2218	0.40	0/2998
3	E	0.63	0/365	0.88	0/561
4	F	0.44	0/142	0.75	0/218
5	G	0.42	0/251	0.93	2/384 (0.5%)
All	All	0.29	0/5249	0.51	2/7234 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	36	DA	O4'-C1'-N9	5.16	111.61	108.00
5	G	34	DA	O4'-C1'-N9	5.14	111.60	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	350	ARG	Sidechain

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	2234	0	2274	21	0
2	B	2187	0	2222	27	0
3	E	327	0	183	26	0
4	F	127	0	69	26	0
5	G	224	0	124	4	0
6	A	1	0	0	0	0
7	A	21	0	0	2	0
7	B	18	0	0	4	0
7	E	4	0	0	2	0
7	F	1	0	0	0	0
7	G	3	0	0	1	0
All	All	5147	0	4872	95	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 10.

All (95) 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)
3:E:11:DC:C6	3:E:12:DT:H72	1.53	1.42
4:F:23:DA:H2'	4:F:24:DT:C7	1.48	1.39
4:F:23:DA:C2'	4:F:24:DT:H72	1.69	1.23
4:F:23:DA:C2'	4:F:24:DT:C7	2.16	1.23
3:E:7:DG:H2'	3:E:8:DT:H72	1.15	1.08
4:F:23:DA:H2'	4:F:24:DT:H73	1.39	1.03
2:B:342:THR:O	7:B:618:HOH:O	1.74	1.03
4:F:23:DA:H2'	4:F:24:DT:H72	1.05	1.02
3:E:7:DG:C2'	3:E:8:DT:H72	1.92	0.99
3:E:11:DC:C6	3:E:12:DT:C7	2.46	0.98
2:B:342:THR:C	7:B:618:HOH:O	2.00	0.97
3:E:7:DG:H2'	3:E:8:DT:C7	1.97	0.95
4:F:24:DT:H6	4:F:24:DT:H5"	1.28	0.94
3:E:8:DT:C5'	3:E:8:DT:H6	1.82	0.92
4:F:23:DA:C2'	4:F:24:DT:H73	1.93	0.92
5:G:38:DT:H73	7:G:103:HOH:O	0.75	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:25:DT:H2"	4:F:26:DG:O5'	1.69	0.91
4:F:24:DT:C6	4:F:24:DT:H5"	2.06	0.90
3:E:6:DT:OP2	7:E:103:HOH:O	1.90	0.89
2:B:345:GLY:N	7:B:618:HOH:O	1.88	0.88
4:F:23:DA:H2"	4:F:24:DT:O5'	1.74	0.87
4:F:24:DT:C5'	4:F:24:DT:H6	1.88	0.85
3:E:11:DC:C5	3:E:12:DT:H72	2.13	0.83
4:F:23:DA:N9	4:F:24:DT:H72	1.95	0.82
4:F:23:DA:C1'	4:F:24:DT:H72	2.14	0.78
4:F:24:DT:H2"	4:F:25:DT:O5'	1.86	0.75
4:F:23:DA:C8	4:F:24:DT:H72	2.22	0.74
1:A:317:PRO:O	7:A:701:HOH:O	2.09	0.71
3:E:8:DT:C5'	3:E:8:DT:C6	2.72	0.70
3:E:11:DC:C5	3:E:12:DT:C7	2.74	0.70
4:F:23:DA:H2"	4:F:24:DT:H73	1.73	0.69
3:E:8:DT:H6	3:E:8:DT:H5'	1.55	0.69
4:F:23:DA:H2"	4:F:24:DT:C7	2.18	0.68
2:B:309:GLU:O	2:B:357:LYS:NZ	2.28	0.66
4:F:25:DT:H4'	4:F:26:DG:OP1	1.94	0.66
3:E:8:DT:H5"	3:E:8:DT:H6	1.62	0.65
3:E:7:DG:H2"	3:E:8:DT:H5"	1.78	0.64
3:E:7:DG:C2'	3:E:8:DT:C7	2.68	0.64
4:F:24:DT:C5'	4:F:24:DT:C6	2.76	0.63
3:E:8:DT:H2'	3:E:9:DG:O4'	2.00	0.61
3:E:6:DT:H3	5:G:34:DA:H61	1.48	0.61
3:E:8:DT:H5"	3:E:8:DT:C6	2.38	0.58
4:F:23:DA:C2'	4:F:24:DT:O5'	2.51	0.57
3:E:11:DC:N1	3:E:12:DT:H72	2.10	0.57
2:B:483:ARG:HA	2:B:501:VAL:HG21	1.85	0.57
3:E:8:DT:H2"	7:E:104:HOH:O	2.07	0.55
2:B:291:VAL:HG13	2:B:313:LEU:HB3	1.88	0.55
3:E:8:DT:H2'	3:E:9:DG:C8	2.42	0.54
1:A:499:THR:HG21	2:B:560:LEU:HA	1.89	0.54
2:B:354:THR:HB	2:B:357:LYS:HD2	1.91	0.53
1:A:350:ARG:HD3	2:B:461:LEU:CD1	2.39	0.53
1:A:392:GLN:NE2	2:B:422:GLN:HG2	2.24	0.53
1:A:338:ASP:OD1	1:A:339:ASP:N	2.42	0.52
1:A:360:GLY:O	7:A:721:HOH:O	2.19	0.52
4:F:25:DT:H2'	4:F:26:DG:N9	2.25	0.52
3:E:8:DT:C2'	3:E:9:DG:O4'	2.58	0.52
1:A:486:SER:OG	5:G:34:DA:OP1	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:24:DT:H2"	4:F:25:DT:C5'	2.40	0.52
2:B:446:ALA:HB3	2:B:447:PRO:HD3	1.92	0.52
1:A:472:ARG:HB2	2:B:562:PRO:HB2	1.91	0.52
2:B:347:VAL:HG21	2:B:415:LEU:HD11	1.93	0.51
4:F:25:DT:H2'	4:F:26:DG:C8	2.46	0.51
2:B:490:ASN:O	2:B:552:ARG:NH2	2.44	0.51
1:A:402:THR:HG23	1:A:407:GLU:HB2	1.92	0.51
1:A:394:ILE:HD13	2:B:449:LYS:HD2	1.94	0.49
2:B:459:PHE:HA	2:B:462:GLU:HB2	1.94	0.48
2:B:325:ILE:HD11	2:B:403:VAL:HG11	1.96	0.48
2:B:256:LEU:HD23	2:B:291:VAL:HB	1.96	0.48
2:B:362:VAL:HG11	2:B:432:LEU:HD23	1.97	0.47
2:B:483:ARG:NH1	2:B:487:GLN:OE1	2.48	0.46
2:B:483:ARG:NH1	2:B:494:LEU:HD12	2.30	0.46
4:F:25:DT:H2"	4:F:26:DG:O4'	2.16	0.45
3:E:6:DT:H2'	3:E:7:DG:C8	2.51	0.45
1:A:527:ARG:HD3	1:A:530:ARG:HB2	1.99	0.45
3:E:14:DA:H2'	3:E:15:DA:C8	2.51	0.45
1:A:308:PHE:HB2	1:A:332:VAL:HB	1.98	0.44
1:A:304:HIS:O	1:A:355:ARG:NH2	2.49	0.44
1:A:471:VAL:HG21	2:B:559:THR:HG21	1.99	0.44
2:B:260:LEU:HB2	2:B:289:CYS:HA	1.99	0.44
2:B:345:GLY:CA	7:B:618:HOH:O	2.52	0.43
1:A:499:THR:OG1	1:A:500:PRO:HD2	2.18	0.43
2:B:315:LEU:HD23	2:B:316:LEU:N	2.34	0.43
3:E:11:DC:C5	3:E:12:DT:H71	2.52	0.42
1:A:275:ILE:O	1:A:275:ILE:HG23	2.18	0.42
2:B:329:LYS:NZ	2:B:414:ASP:OD2	2.46	0.42
4:F:25:DT:C2'	4:F:26:DG:O4'	2.67	0.42
5:G:29:DG:H2'	5:G:30:DA:C8	2.55	0.41
1:A:475:PHE:CD1	1:A:500:PRO:HG3	2.55	0.41
3:E:11:DC:H2'	3:E:12:DT:H72	2.02	0.41
4:F:23:DA:H4'	4:F:24:DT:OP1	2.21	0.41
1:A:479:LEU:HA	1:A:479:LEU:HD12	1.94	0.41
1:A:350:ARG:HD3	2:B:461:LEU:HD11	2.03	0.41
1:A:528:LEU:HA	1:A:529:GLN:HA	1.76	0.41
3:E:5:DG:C8	3:E:6:DT:H72	2.57	0.40
1:A:400:LYS:HG3	1:A:411:TYR: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	277/306 (90%)	269 (97%)	6 (2%)	2 (1%)	26	62
2	B	270/393 (69%)	256 (95%)	13 (5%)	1 (0%)	39	74
All	All	547/699 (78%)	525 (96%)	19 (4%)	3 (0%)	34	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	432	PRO
2	B	245	PRO
1	A	259	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	244/259 (94%)	231 (95%)	13 (5%)	28	61
2	B	238/334 (71%)	221 (93%)	17 (7%)	18	46
All	All	482/593 (81%)	452 (94%)	30 (6%)	23	54

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	ARG
1	A	269	VAL
1	A	274	ASP

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Mol	Chain	Res	Type
1	A	364	ARG
1	A	375	HIS
1	A	422	LEU
1	A	454	LEU
1	A	465	LYS
1	A	479	LEU
1	A	482	VAL
1	A	483	ARG
1	A	527	ARG
1	A	543	LEU
2	B	240	MET
2	B	244	ARG
2	B	249	LEU
2	B	269	LEU
2	B	273	LEU
2	B	285	GLN
2	B	291	VAL
2	B	302	ASP
2	B	319	GLU
2	B	342	THR
2	B	343	LEU
2	B	412	LEU
2	B	459	PHE
2	B	461	LEU
2	B	472	ASP
2	B	531	GLN
2	B	534	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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(Å²)	Q<0.9
1	A	283/306 (92%)	0.50	16 (5%)	27	17	36, 66, 112, 154	0
2	B	278/393 (70%)	0.59	23 (8%)	14	7	44, 70, 131, 157	0
3	E	16/17 (94%)	1.16	5 (31%)	1	0	68, 119, 153, 160	0
4	F	6/6 (100%)	1.68	2 (33%)	0	0	135, 139, 143, 146	0
5	G	11/16 (68%)	1.43	2 (18%)	2	1	110, 122, 136, 137	0
All	All	594/738 (80%)	0.59	48 (8%)	15	7	36, 70, 132, 160	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	528	LEU	13.7
2	B	242	ALA	7.7
2	B	302	ASP	7.3
2	B	243	GLN	7.0
2	B	299	PRO	5.8
1	A	529	GLN	5.5
1	A	256	GLN	5.4
2	B	301	GLU	5.2
1	A	257	GLN	4.3
2	B	461	LEU	4.3
2	B	300	SER	4.1
2	B	297	ALA	4.0
5	G	33	DC	4.0
1	A	375	HIS	3.9
2	B	245	PRO	3.8
1	A	372	GLY	3.7
1	A	435	THR	3.5
1	A	374	VAL	3.4
3	E	12	DT	3.4
3	E	14	DA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	532	LEU	3.3
1	A	285	PRO	3.3
2	B	458	SER	3.3
2	B	459	PHE	3.1
2	B	303	ARG	3.0
2	B	369	CYS	3.0
2	B	298	GLY	2.9
2	B	534	ARG	2.9
2	B	460	CYS	2.8
5	G	32	DA	2.8
1	A	280	GLY	2.8
4	F	26	DG	2.8
2	B	306	TRP	2.6
2	B	241	LYS	2.6
4	F	23	DA	2.6
3	E	13	DC	2.6
1	A	483	ARG	2.5
1	A	547	TYR	2.4
3	E	17	DC	2.4
2	B	457	PHE	2.4
2	B	329	LYS	2.3
1	A	482	VAL	2.3
2	B	308	GLU	2.3
3	E	7	DG	2.2
1	A	295	HIS	2.2
2	B	279	ARG	2.2
1	A	484	GLY	2.1
2	B	296	ARG	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
6	MG	A	601	1/1	0.63	0.16	-	76,76,76,76	0

6.5 Other polymers (i)

There are no such residues in this entry.