



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:27 PM GMT

PDB ID : 4F0Q  
Title : MspJI Restriction Endonuclease - P21 Form  
Authors : Horton, J.R.; Mabuchi, M.; Cohen-Karni, D.; Zhang, X.; Griggs, R.; Samaranyake, M.; Roberts, R.J.; Zheng, Y.; Cheng, X.  
Deposited on : 2012-05-04  
Resolution : 2.05 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

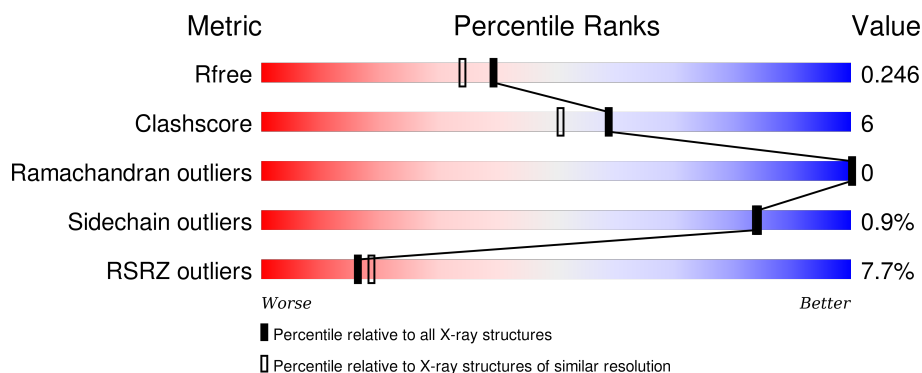
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	456	<div> <div>3%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	B	456	<div> <div>6%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	C	456	<div> <div>10%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	D	456	<div> <div>11%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14351 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 Restriction endonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	1	0
			3440	2160	644	631	5			
1	B	452	Total	C	N	O	S	0	0	0
			3386	2124	630	627	5			
1	C	449	Total	C	N	O	S	0	0	0
			3284	2064	609	607	4			
1	D	447	Total	C	N	O	S	0	1	0
			3249	2036	606	602	5			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

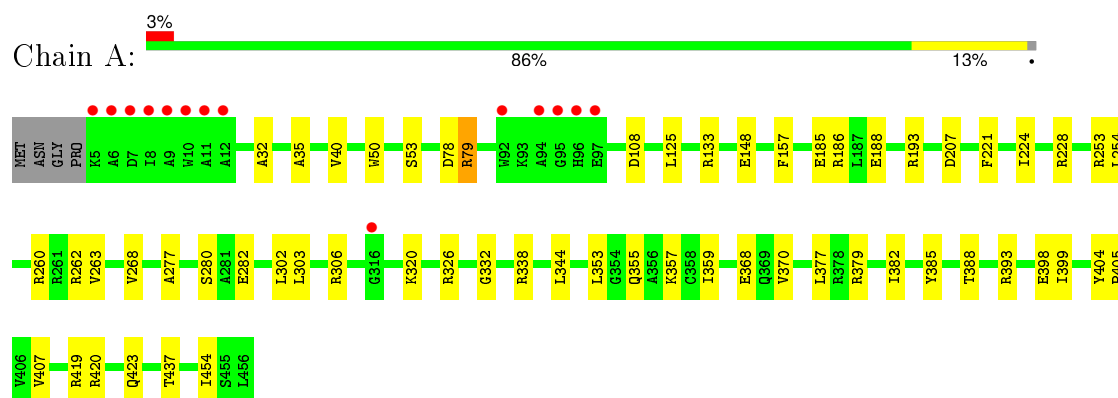
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	334	Total	O	0	0
			334	334		
3	B	271	Total	O	0	0
			271	271		
3	C	215	Total	O	0	0
			215	215		
3	D	169	Total	O	0	0
			169	169		

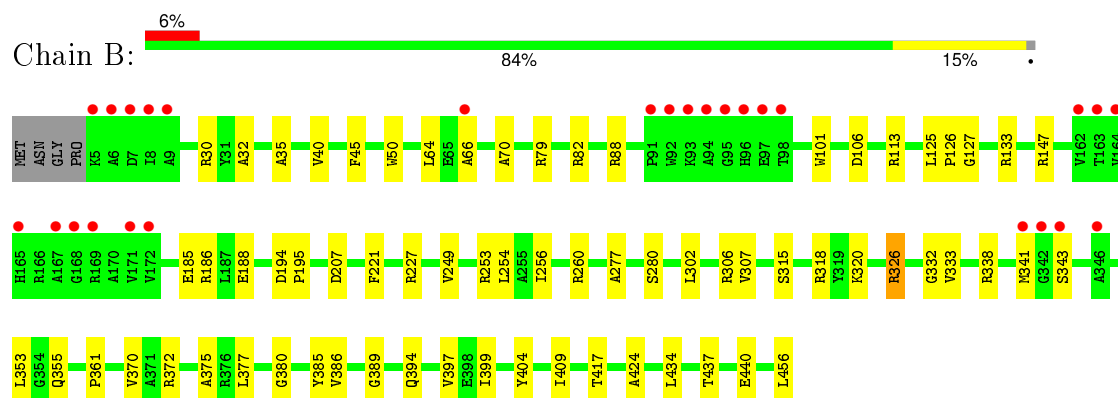
### 3 Residue-property plots

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.

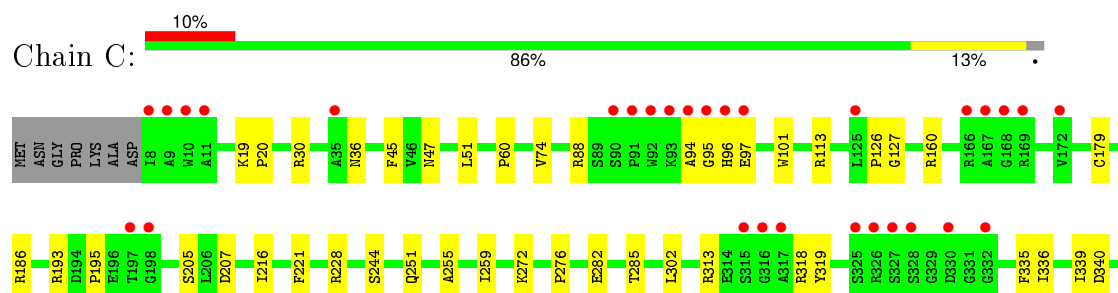
#### • Molecule 1: Restriction endonuclease

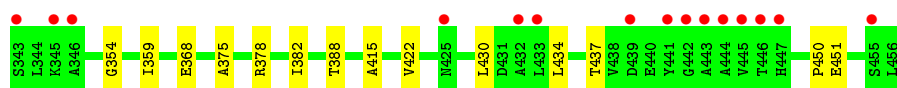


#### • Molecule 1: Restriction endonuclease

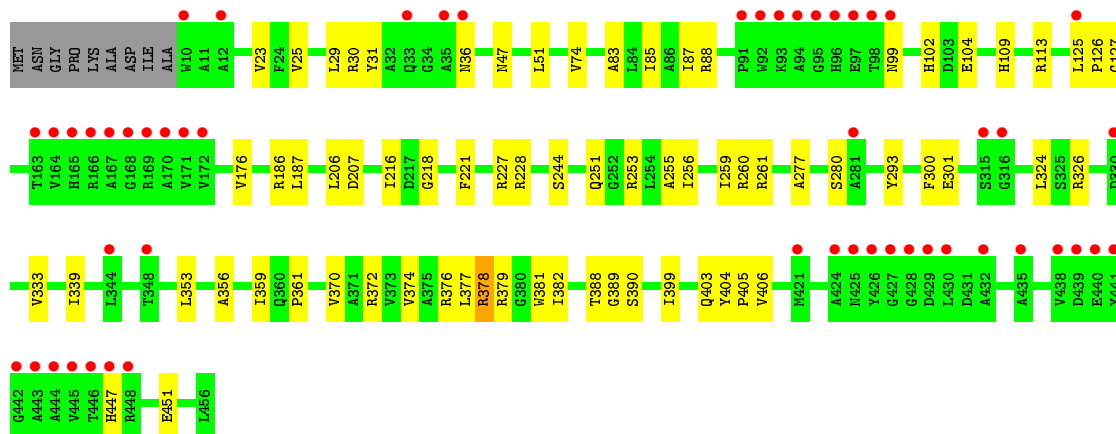
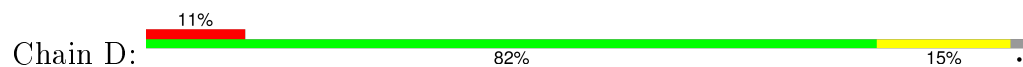


#### • Molecule 1: Restriction endonuclease





● Molecule 1: Restriction endonuclease



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.76Å 144.28Å 87.84Å 90.00° 116.27° 90.00°	Depositor
Resolution (Å)	34.57 – 2.05 34.57 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.57-2.05) 97.6 (34.57-2.05)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.59 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.210 , 0.246 0.209 , 0.246	Depositor DCC
$R_{free}$ test set	6064 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 25.2	EDS
Estimated twinning fraction	0.377 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 122216 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14351	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	0.20	0/3516	0.37	0/4777
1	B	0.21	0/3455	0.38	0/4699
1	C	0.21	0/3350	0.38	0/4566
1	D	0.21	0/3318	0.39	0/4522
All	All	0.21	0/13639	0.38	0/18564

There are no bond length outliers.

There are no bond angle outliers.

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	3440	0	3393	42	0
1	B	3386	0	3300	44	0
1	C	3284	0	3138	38	0
1	D	3249	0	3064	47	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	334	0	0	3	0
3	B	271	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	215	0	0	4	0
3	D	169	0	0	4	0
All	All	14351	0	12895	152	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 (152) 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:D:125:LEU:HG	1:D:126:PRO:HD2	1.66	0.74
1:C:186:ARG:HB3	1:C:207:ASP:HB2	1.71	0.73
1:D:244:SER:HB2	1:D:259:ILE:HB	1.71	0.72
1:A:254:LEU:HD23	1:B:306:ARG:HD3	1.77	0.66
1:A:379:ARG:NH2	1:C:375:ALA:O	2.29	0.65
1:A:368:GLU:HG3	1:D:372:ARG:HD2	1.79	0.65
1:D:125:LEU:CG	1:D:126:PRO:HD2	2.26	0.65
1:D:99:ASN:O	1:D:102:HIS:ND1	2.31	0.64
1:C:113:ARG:NH1	3:C:729:HOH:O	2.31	0.63
1:B:277:ALA:HB3	1:B:280:SER:HB3	1.81	0.63
1:A:32:ALA:HB3	1:A:35:ALA:HB2	1.80	0.62
1:A:133:ARG:HG3	1:B:125:LEU:HD11	1.82	0.62
1:C:451:GLU:OE1	1:D:403:GLN:NE2	2.33	0.62
1:D:339:ILE:HD12	1:D:382:ILE:HD11	1.82	0.61
1:D:359:ILE:O	1:D:388:THR:OG1	2.19	0.60
1:A:253:ARG:NH1	3:A:908:HOH:O	2.33	0.60
1:A:382:ILE:HD13	1:B:341:MET:HE3	1.84	0.60
1:B:66:ALA:HB2	1:B:88:ARG:HH21	1.65	0.59
1:B:320:LYS:HE2	1:B:456:LEU:HB3	1.83	0.59
1:A:332:GLY:O	1:A:355:GLN:NE2	2.36	0.58
1:B:375:ALA:O	1:D:379:ARG:NH2	2.37	0.58
1:D:113:ARG:NH1	3:D:588:HOH:O	2.35	0.58
1:D:326:ARG:NH2	1:D:333:VAL:O	2.32	0.58
1:A:188:GLU:HA	1:B:188:GLU:HA	1.87	0.57
1:C:359:ILE:O	1:C:388:THR:OG1	2.22	0.57
1:D:293:TYR:HB3	1:D:300:PHE:HB2	1.87	0.57
1:A:277:ALA:HB3	1:A:280:SER:HB3	1.87	0.56
1:A:302:LEU:HD23	1:A:437:THR:HA	1.88	0.56
1:D:186:ARG:HB3	1:D:207:ASP:HB2	1.89	0.55
1:A:407:VAL:HG13	1:B:343:SER:HB2	1.88	0.55
1:D:125:LEU:CD1	1:D:126:PRO:HD2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:VAL:HG21	1:C:228:ARG:HA	1.89	0.55
1:C:422:VAL:HG21	1:C:430:LEU:HA	1.89	0.54
1:B:302:LEU:HD23	1:B:437:THR:HA	1.88	0.54
1:B:399:ILE:HG23	1:B:404:TYR:HB2	1.91	0.53
1:B:70:ALA:HB1	1:B:82:ARG:HD2	1.91	0.52
1:B:40:VAL:HG12	1:B:50:TRP:CE2	2.45	0.52
1:C:313:ARG:NH1	1:C:319:TYR:O	2.43	0.52
1:D:30:ARG:NH1	1:D:31:TYR:O	2.43	0.52
1:D:36:ASN:O	1:D:47:ASN:ND2	2.43	0.52
1:A:78:ASP:OD2	1:A:79:ARG:NH1	2.43	0.52
1:C:30:ARG:HG2	1:C:45:PHE:HB2	1.92	0.52
1:C:276:PRO:HB3	1:C:282:GLU:HG3	1.92	0.51
1:D:29:LEU:HB2	1:D:176:VAL:HG23	1.91	0.51
1:D:251:GLN:HB2	1:D:255:ALA:HB2	1.93	0.51
1:A:359:ILE:O	1:A:388:THR:OG1	2.28	0.51
1:B:253:ARG:HD3	1:B:256:ILE:HD12	1.93	0.51
1:C:244:SER:HB2	1:C:259:ILE:HB	1.94	0.50
1:A:306:ARG:HD3	1:B:254:LEU:HD13	1.92	0.50
1:A:379:ARG:NH1	3:A:804:HOH:O	2.39	0.50
1:D:23:VAL:HB	1:D:51:LEU:HD21	1.94	0.49
1:D:125:LEU:HD12	1:D:126:PRO:HD2	1.95	0.49
1:C:113:ARG:HE	1:C:205:SER:HG	1.59	0.49
1:D:253:ARG:HH11	1:D:256:ILE:HD12	1.77	0.48
1:B:30:ARG:HB2	1:B:45:PHE:HB2	1.95	0.48
1:D:187:LEU:HD12	1:D:206:LEU:HD11	1.95	0.48
1:A:108:ASP:OD2	1:C:193:ARG:NH1	2.47	0.48
1:B:372:ARG:HD2	1:C:368:GLU:HG3	1.96	0.48
1:D:370:VAL:HG11	1:D:399:ILE:HD11	1.94	0.48
1:C:160:ARG:NH1	1:C:179:CYS:SG	2.81	0.48
1:B:64:LEU:HG	1:B:88:ARG:HB2	1.96	0.48
1:D:374:VAL:HG22	1:D:406:VAL:HG21	1.96	0.48
1:A:357:LYS:HG2	1:A:359:ILE:HG23	1.95	0.48
1:D:88:ARG:NH2	3:D:517:HOH:O	2.46	0.48
1:D:216:ILE:HG13	1:D:218:GLY:H	1.79	0.47
1:B:82:ARG:O	1:B:227:ARG:NH2	2.43	0.47
1:B:332:GLY:O	1:B:355:GLN:NE2	2.47	0.47
1:B:306:ARG:NH2	1:B:440:GLU:OE1	2.47	0.47
1:A:399:ILE:HG23	1:A:404:TYR:HB2	1.96	0.47
1:B:260:ARG:NH1	3:B:673:HOH:O	2.44	0.47
1:B:147:ARG:HG3	1:B:249:VAL:HG12	1.97	0.46
1:C:36:ASN:O	1:C:47:ASN:ND2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:NH2	1:A:148:GLU:O	2.49	0.46
1:B:186:ARG:NH1	1:B:315:SER:O	2.45	0.46
1:C:251:GLN:HB2	1:C:255:ALA:HB2	1.97	0.46
1:A:320:LYS:HG3	1:A:338:ARG:HH21	1.80	0.45
1:B:101:TRP:HZ2	1:B:424:ALA:HB2	1.81	0.45
1:B:32:ALA:HB3	1:B:35:ALA:HB2	1.98	0.45
1:D:51:LEU:HG	1:D:221:PHE:CD2	2.52	0.45
1:C:101:TRP:HH2	1:C:195:PRO:HD3	1.82	0.45
1:C:339:ILE:HD12	1:C:382:ILE:HD11	1.99	0.45
1:B:386:VAL:HG22	1:B:409:ILE:HD12	1.98	0.45
1:D:102:HIS:NE2	1:D:104:GLU:OE1	2.50	0.44
1:B:370:VAL:HG11	1:B:399:ILE:HD11	1.99	0.44
1:C:336:ILE:HD13	1:C:450:PRO:HA	1.98	0.44
1:B:394:GLN:HA	1:B:397:VAL:HG22	1.99	0.44
1:C:318:ARG:HB2	1:C:340:ASP:HB2	1.99	0.44
1:A:398:GLU:CD	1:D:376:ARG:HH22	2.20	0.44
1:D:256:ILE:HA	1:D:259:ILE:HG12	1.98	0.44
1:D:74:VAL:HG21	1:D:228:ARG:HA	1.99	0.44
1:A:282:GLU:HG2	1:A:419:ARG:HD3	2.00	0.44
1:C:302:LEU:HD23	1:C:437:THR:HA	1.98	0.44
1:A:193:ARG:NH1	1:A:423:GLN:OE1	2.49	0.44
1:C:95:GLY:HA2	1:C:96:HIS:C	2.38	0.44
1:C:430:LEU:HG	1:C:434:LEU:HG	1.99	0.43
1:C:51:LEU:HG	1:C:221:PHE:CD2	2.53	0.43
1:B:353:LEU:HD22	1:B:377:LEU:HD23	1.99	0.43
1:D:399:ILE:HG23	1:D:404:TYR:HB2	2.00	0.43
1:C:282:GLU:HB2	1:C:415:ALA:HB1	2.00	0.43
1:A:370[A]:VAL:HG11	1:A:399:ILE:HD11	2.01	0.43
1:A:405:PRO:HB3	1:B:380:GLY:HA3	2.00	0.43
1:C:94:ALA:HB2	1:D:447:HIS:HA	2.00	0.43
1:D:301:GLU:HG2	1:D:356:ALA:HB3	1.99	0.43
1:C:378:ARG:NH2	3:C:624:HOH:O	2.51	0.43
1:B:320:LYS:HB3	1:B:338:ARG:HB3	2.00	0.43
1:D:377:LEU:HD13	1:D:405:PRO:HG2	2.00	0.43
1:B:326:ARG:NH2	1:B:333:VAL:O	2.38	0.43
1:B:361:PRO:HA	1:B:389:GLY:HA2	2.01	0.43
1:B:185:GLU:OE1	1:B:260:ARG:NH1	2.52	0.43
1:D:370:VAL:O	1:D:374:VAL:HG23	2.19	0.43
1:D:361:PRO:HA	1:D:389:GLY:HA2	2.00	0.43
1:C:126:PRO:HA	1:C:127:GLY:HA2	1.57	0.43
1:A:40:VAL:HG12	1:A:50:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:PRO:HA	1:B:127:GLY:HA2	1.49	0.42
1:D:353:LEU:HD12	1:D:377:LEU:HD23	2.01	0.42
1:A:268:VAL:HG11	1:A:393:ARG:HG3	2.01	0.42
1:B:434:LEU:O	1:B:437:THR:OG1	2.29	0.42
1:A:78:ASP:OD1	1:A:78:ASP:N	2.51	0.42
1:B:194:ASP:HA	1:B:195:PRO:HD3	1.89	0.42
1:B:186:ARG:HB3	1:B:207:ASP:HB2	2.02	0.42
1:A:125:LEU:HD11	1:B:133:ARG:HG3	2.01	0.42
1:A:157:PHE:CE1	1:A:224:ILE:HD11	2.55	0.42
1:D:228:ARG:NH2	3:D:598:HOH:O	2.43	0.42
1:D:378:ARG:NH2	3:D:622:HOH:O	2.53	0.42
1:D:126:PRO:HA	1:D:127:GLY:HA2	1.35	0.42
1:C:272:LYS:HB3	1:C:272:LYS:HE2	1.83	0.42
1:C:60:PRO:O	1:C:228:ARG:NH2	2.37	0.41
1:C:251:GLN:NE2	3:C:714:HOH:O	2.43	0.41
1:B:79:ARG:NH2	3:B:680:HOH:O	2.53	0.41
1:D:83:ALA:O	1:D:227:ARG:NE	2.39	0.41
1:C:19:LYS:HA	1:C:20:PRO:HD3	1.91	0.41
1:D:381:TRP:HZ2	1:D:451:GLU:HB3	1.86	0.41
1:C:88:ARG:NH2	3:C:781:HOH:O	2.37	0.41
1:A:420:ARG:NH2	3:A:844:HOH:O	2.53	0.41
1:C:95:GLY:HA2	1:C:97:GLU:N	2.36	0.41
1:A:379:ARG:HH22	1:C:375:ALA:C	2.23	0.41
1:D:109:HIS:O	1:D:260:ARG:HD3	2.20	0.41
1:B:307:VAL:HG13	1:B:417:THR:HG21	2.02	0.41
1:A:53:SER:HB2	1:A:228:ARG:HH12	1.85	0.41
1:C:335:PHE:CE1	1:C:354:GLY:HA3	2.56	0.41
1:A:353:LEU:HD22	1:A:377:LEU:HD23	2.02	0.41
1:A:344:LEU:HD13	1:B:113:ARG:HG3	2.03	0.40
1:A:303:LEU:HB2	1:A:437:THR:HG21	2.03	0.40
1:C:282:GLU:HA	1:C:285:THR:HB	2.03	0.40
1:D:25:VAL:HG11	1:D:261:ARG:NH1	2.37	0.40
1:A:185:GLU:CD	1:A:260:ARG:HH12	2.25	0.40
1:A:338:ARG:NH1	1:A:454:ILE:O	2.54	0.40
1:A:186:ARG:HB3	1:A:207:ASP:HB2	2.04	0.40
1:A:262:ARG:NH1	1:A:263:VAL:O	2.54	0.40
1:A:344:LEU:HD21	1:B:106:ASP:HB2	2.04	0.40
1:D:277:ALA:HB3	1:D:280:SER:OG	2.22	0.40
1:D:85:ILE:HG22	1:D:87:ILE:HG13	2.03	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	451/456 (99%)	440 (98%)	11 (2%)	0	100	100
1	B	450/456 (99%)	433 (96%)	17 (4%)	0	100	100
1	C	447/456 (98%)	421 (94%)	26 (6%)	0	100	100
1	D	446/456 (98%)	427 (96%)	19 (4%)	0	100	100
All	All	1794/1824 (98%)	1721 (96%)	73 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/358 (96%)	340 (99%)	4 (1%)	78	76
1	B	332/358 (93%)	328 (99%)	4 (1%)	78	76
1	C	308/358 (86%)	307 (100%)	1 (0%)	94	95
1	D	299/358 (84%)	296 (99%)	3 (1%)	82	81
All	All	1283/1432 (90%)	1271 (99%)	12 (1%)	84	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
1	A	221	PHE

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Mol	Chain	Res	Type
1	A	326	ARG
1	A	385	TYR
1	B	221	PHE
1	B	318	ARG
1	B	326	ARG
1	B	385	TYR
1	C	216	ILE
1	D	324	LEU
1	D	378	ARG
1	D	390	SER

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	452/456 (99%)	0.15	14 (3%) 52 60	13, 22, 38, 78	0
1	B	452/456 (99%)	0.28	27 (5%) 25 28	11, 23, 51, 79	0
1	C	449/456 (98%)	0.67	45 (10%) 9 10	17, 30, 64, 105	0
1	D	447/456 (98%)	0.94	52 (11%) 6 7	16, 32, 76, 126	0
All	All	1800/1824 (98%)	0.51	138 (7%) 16 19	11, 26, 60, 126	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	TRP	25.8
1	D	95	GLY	17.6
1	D	92	TRP	17.6
1	C	446	THR	17.3
1	D	96	HIS	16.4
1	C	95	GLY	15.9
1	C	441	TYR	14.6
1	A	5	LYS	12.9
1	C	442	GLY	12.4
1	D	447	HIS	12.3
1	B	94	ALA	11.5
1	C	96	HIS	11.5
1	A	94	ALA	11.3
1	D	427	GLY	11.3
1	B	92	TRP	10.8
1	D	164	VAL	10.4
1	D	171	VAL	10.2
1	C	167	ALA	9.9
1	D	426	TYR	9.8
1	D	91	PRO	9.5
1	D	94	ALA	9.3

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Mol	Chain	Res	Type	RSRZ
1	D	441	TYR	9.3
1	D	444	ALA	8.7
1	D	428	GLY	8.4
1	D	168	GLY	8.4
1	B	168	GLY	8.1
1	A	8	ILE	7.5
1	D	166	ARG	7.4
1	C	445	VAL	7.4
1	C	166	ARG	7.3
1	C	447	HIS	7.2
1	D	445	VAL	7.2
1	D	170	ALA	7.1
1	D	35	ALA	6.8
1	C	346	ALA	6.4
1	D	169	ARG	6.4
1	D	98	THR	6.3
1	D	97	GLU	6.2
1	B	95	GLY	6.1
1	D	165	HIS	6.1
1	C	90	SER	6.1
1	C	92	TRP	6.0
1	D	10	TRP	5.9
1	C	94	ALA	5.7
1	A	95	GLY	5.6
1	B	96	HIS	5.6
1	C	443	ALA	5.6
1	C	168	GLY	5.5
1	B	342	GLY	5.5
1	C	91	PRO	5.3
1	C	8	ILE	5.2
1	D	443	ALA	5.2
1	B	162	VAL	5.2
1	D	167	ALA	5.2
1	C	316	GLY	5.1
1	B	346	ALA	5.0
1	B	93	LYS	5.0
1	B	167	ALA	4.8
1	B	6	ALA	4.7
1	D	442	GLY	4.7
1	B	164	VAL	4.7
1	D	432	ALA	4.6
1	D	440	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	96	HIS	4.5
1	B	343	SER	4.4
1	D	446	THR	4.2
1	C	9	ALA	4.2
1	C	317	ALA	4.2
1	B	8	ILE	4.2
1	B	98	THR	4.1
1	B	169	ARG	4.0
1	C	325	SER	4.0
1	C	332	GLY	4.0
1	B	66	ALA	3.9
1	C	315	SER	3.9
1	B	165	HIS	3.9
1	D	429	ASP	3.9
1	C	345	LYS	3.9
1	A	6	ALA	3.8
1	A	7	ASP	3.7
1	D	163	THR	3.7
1	A	316	GLY	3.7
1	D	438	VAL	3.6
1	C	10	TRP	3.5
1	D	36	ASN	3.5
1	D	344	LEU	3.3
1	C	444	ALA	3.3
1	B	5	LYS	3.3
1	B	91	PRO	3.3
1	C	169	ARG	3.2
1	B	97	GLU	3.2
1	B	172	VAL	3.1
1	D	315	SER	3.1
1	C	97	GLU	3.1
1	D	330	ASP	3.1
1	D	93	LYS	3.0
1	C	172	VAL	2.9
1	B	163	THR	2.8
1	D	448	ARG	2.8
1	A	9	ALA	2.8
1	D	172	VAL	2.8
1	C	11	ALA	2.8
1	D	316	GLY	2.8
1	C	93	LYS	2.8
1	D	421	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	439	ASP	2.7
1	C	330	ASP	2.7
1	B	9	ALA	2.6
1	D	424	ALA	2.6
1	D	348	THR	2.6
1	C	328	SER	2.6
1	D	435	ALA	2.6
1	C	327	SER	2.5
1	D	430	LEU	2.5
1	C	326	ARG	2.5
1	D	439	ASP	2.5
1	C	35	ALA	2.4
1	A	12	ALA	2.3
1	C	455	SER	2.3
1	D	425	ASN	2.3
1	B	7	ASP	2.3
1	D	99	ASN	2.3
1	C	125	LEU	2.3
1	A	97	GLU	2.2
1	A	11	ALA	2.2
1	C	343	SER	2.2
1	B	171	VAL	2.2
1	D	281	ALA	2.2
1	A	10	TRP	2.1
1	C	197	THR	2.1
1	D	33	GLN	2.1
1	C	433	LEU	2.1
1	D	12	ALA	2.1
1	C	198	GLY	2.0
1	D	125	LEU	2.0
1	B	341	MET	2.0
1	C	432	ALA	2.0
1	C	425	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	MG	A	501	1/1	0.96	0.07	-1.68	21,21,21,21	0
2	MG	B	501	1/1	0.97	0.07	-2.16	19,19,19,19	0
2	MG	C	501	1/1	0.95	0.07	-2.93	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.