



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 06:08 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 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/ValidationPDFNotes.html>

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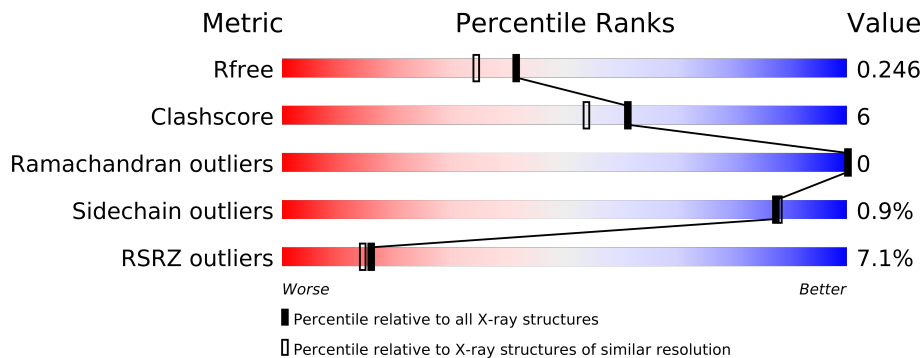
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	456	
1	B	456	
1	C	456	
1	D	456	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14351 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

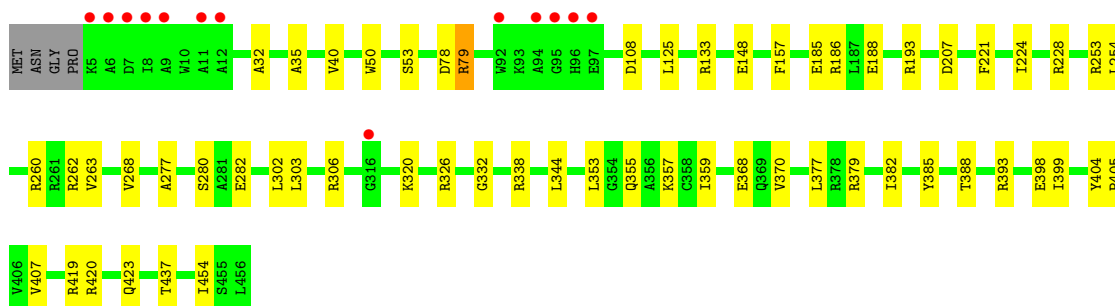
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	334	Total	O	0	0
			334	334		
3	B	271	Total	O	0	0
			271	271		
3	C	215	Total	O	0	0
			215	215		
3	D	169	Total	O	0	0
			169	169		

### 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

Chain A: 



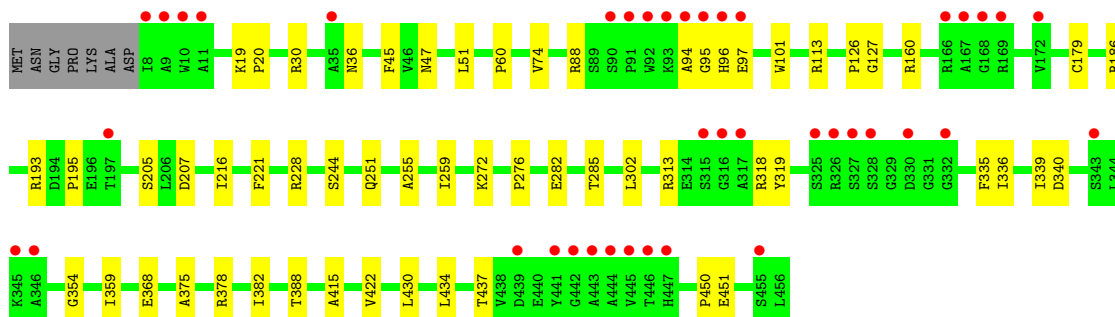
- Molecule 1: Restriction endonuclease

Chain B: 



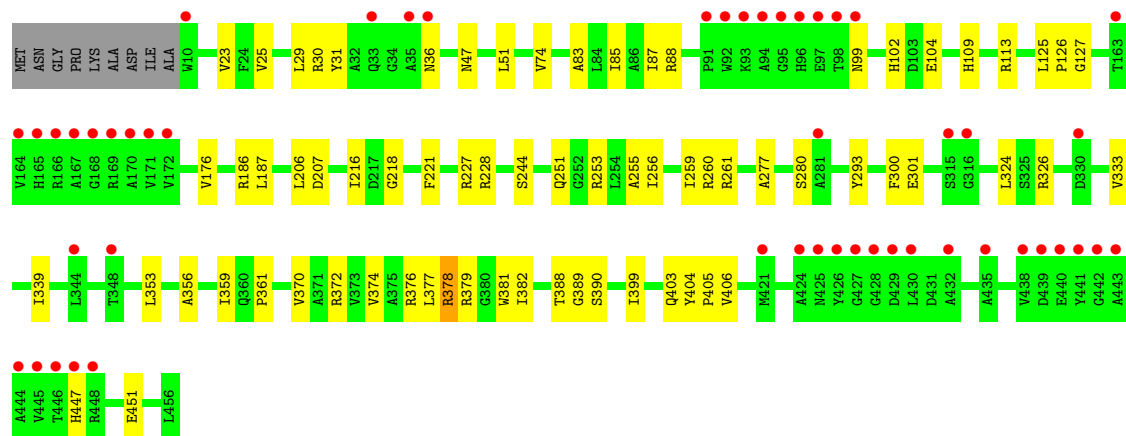
- Molecule 1: Restriction endonuclease

Chain C: 



● Molecule 1: Restriction endonuclease

Chain D: 



## 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> )	0.32 , 26.3	EDS
Estimated twinning fraction	0.377 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	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.

## 5 Model quality

### 5.1 Standard geometry

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 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	271	0	0	2	0
3	C	215	0	0	4	0
3	D	169	0	0	4	0
All	All	14351	0	12895	152	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (152) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:C:74:VAL:HG21	1:C:228:ARG:HA	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

### 5.3.1 Protein backbone ⓘ

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 ⓘ

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%)	82	81
1	B	332/358 (93%)	328 (99%)	4 (1%)	82	81
1	C	308/358 (86%)	307 (100%)	1 (0%)	96	96
1	D	299/358 (84%)	296 (99%)	3 (1%)	85	86
All	All	1283/1432 (90%)	1271 (99%)	12 (1%)	87	88

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

Mol	Chain	Res	Type
1	A	79	ARG
1	A	221	PHE
1	A	326	ARG
1	A	385	TYR
1	B	221	PHE

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Mol	Chain	Res	Type
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 chains 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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	13 (2%)	49	49	13, 22, 38, 78	0
1	B	452/456 (99%)	0.27	25 (5%)	24	23	11, 23, 51, 79	0
1	C	449/456 (98%)	0.63	40 (8%)	10	9	17, 30, 64, 105	0
1	D	447/456 (98%)	0.88	50 (11%)	6	6	16, 32, 76, 126	0
All	All	1800/1824 (98%)	0.48	128 (7%)	16	14	11, 26, 60, 126	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	TRP	21.4
1	D	95	GLY	16.2
1	C	446	THR	16.2
1	C	95	GLY	15.2
1	D	92	TRP	15.0
1	D	96	HIS	14.9
1	C	441	TYR	13.2
1	A	5	LYS	12.0
1	D	447	HIS	11.8
1	C	442	GLY	11.2
1	B	94	ALA	10.8
1	C	96	HIS	10.6
1	D	427	GLY	10.5
1	A	94	ALA	10.3
1	D	164	VAL	9.8
1	D	171	VAL	9.6
1	B	92	TRP	9.3
1	C	167	ALA	9.2
1	D	426	TYR	9.1
1	D	444	ALA	9.0
1	D	94	ALA	8.9

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Mol	Chain	Res	Type	RSRZ
1	D	441	TYR	8.7
1	D	91	PRO	8.5
1	D	168	GLY	7.5
1	D	428	GLY	7.2
1	C	445	VAL	7.2
1	B	168	GLY	7.1
1	A	8	ILE	7.0
1	C	166	ARG	6.9
1	D	166	ARG	6.7
1	D	170	ALA	6.7
1	D	445	VAL	6.5
1	C	447	HIS	6.5
1	D	35	ALA	6.3
1	D	169	ARG	6.2
1	C	346	ALA	6.1
1	D	97	GLU	5.7
1	D	98	THR	5.6
1	D	165	HIS	5.6
1	C	90	SER	5.6
1	B	95	GLY	5.5
1	C	443	ALA	5.5
1	C	94	ALA	5.4
1	B	96	HIS	5.2
1	C	92	TRP	5.2
1	D	10	TRP	5.1
1	A	95	GLY	5.1
1	C	316	GLY	5.1
1	C	168	GLY	5.1
1	B	342	GLY	5.0
1	D	443	ALA	4.9
1	D	167	ALA	4.9
1	B	93	LYS	4.8
1	B	162	VAL	4.8
1	B	346	ALA	4.8
1	D	432	ALA	4.7
1	B	6	ALA	4.7
1	C	91	PRO	4.6
1	C	8	ILE	4.6
1	B	164	VAL	4.6
1	D	442	GLY	4.5
1	D	440	GLU	4.5
1	B	167	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	343	SER	4.3
1	A	96	HIS	4.2
1	C	317	ALA	4.1
1	D	446	THR	4.0
1	C	9	ALA	3.9
1	C	325	SER	3.9
1	C	315	SER	3.8
1	A	6	ALA	3.8
1	A	7	ASP	3.8
1	B	98	THR	3.8
1	B	169	ARG	3.7
1	B	8	ILE	3.7
1	D	438	VAL	3.6
1	D	429	ASP	3.6
1	B	165	HIS	3.6
1	C	345	LYS	3.5
1	B	66	ALA	3.5
1	A	316	GLY	3.5
1	C	332	GLY	3.5
1	D	163	THR	3.4
1	C	444	ALA	3.4
1	D	36	ASN	3.3
1	C	169	ARG	3.2
1	D	315	SER	3.1
1	B	5	LYS	3.0
1	C	97	GLU	3.0
1	B	172	VAL	3.0
1	C	10	TRP	3.0
1	D	344	LEU	3.0
1	B	91	PRO	2.9
1	D	330	ASP	2.9
1	B	97	GLU	2.8
1	D	93	LYS	2.8
1	B	163	THR	2.8
1	C	172	VAL	2.7
1	D	448	ARG	2.7
1	A	9	ALA	2.7
1	C	93	LYS	2.6
1	C	439	ASP	2.6
1	D	439	ASP	2.6
1	B	9	ALA	2.6
1	D	316	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	435	ALA	2.6
1	C	11	ALA	2.6
1	C	330	ASP	2.6
1	D	348	THR	2.6
1	D	421	MET	2.6
1	D	172	VAL	2.5
1	C	328	SER	2.5
1	C	326	ARG	2.4
1	B	7	ASP	2.4
1	A	12	ALA	2.4
1	D	424	ALA	2.3
1	D	430	LEU	2.3
1	A	97	GLU	2.3
1	C	327	SER	2.3
1	C	35	ALA	2.3
1	D	425	ASN	2.3
1	A	11	ALA	2.2
1	C	455	SER	2.2
1	D	99	ASN	2.2
1	C	343	SER	2.1
1	D	33	GLN	2.1
1	D	281	ALA	2.1
1	C	197	THR	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 ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	501	1/1	0.07	-1.89	21,21,21,21	0
2	MG	B	501	1/1	0.06	-2.48	19,19,19,19	0
2	MG	C	501	1/1	0.07	-3.43	33,33,33,33	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.