



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:56 AM GMT

PDB ID : 2A07  
Title : Crystal Structure of Foxp2 bound Specifically to DNA.  
Authors : Stroud, J.C.; Wu, Y.; Bates, D.L.; Han, A.; Nowick, K.; Paabo, S.; Tong, H.;  
Chen, L.  
Deposited on : 2005-06-16  
Resolution : 1.90 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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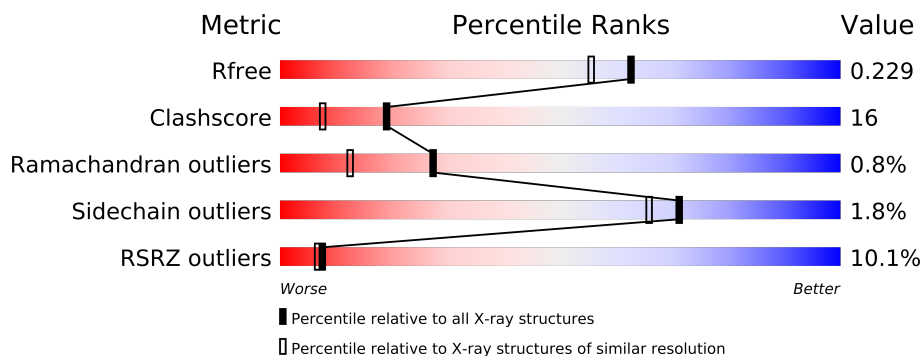
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.90 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	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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	21	
1	C	21	
2	B	21	
2	D	21	
3	F	93	
3	G	93	
3	H	93	
3	I	93	
3	J	93	
3	K	93	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	I	603	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6446 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 DNA chain called 5'-D(\*AP\*AP\*CP\*TP\*AP\*TP\*GP\*AP\*AP\*AP\*CP\*AP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	P	0	0	0
			424	206	76	122	20			
1	C	21	Total	C	N	O	P	0	0	0
			424	206	76	122	20			

- Molecule 2 is a DNA chain called 5'-D(\*TP\*TP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*TP\*GP\*TP\*TP\*TP\*CP\*AP\*TP\*AP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	21	Total	C	N	O	P	0	0	0
			431	209	76	126	20			
2	D	21	Total	C	N	O	P	0	0	0
			431	209	76	126	20			

- Molecule 3 is a protein called Forkhead box protein P2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	82	Total	C	N	O	S	0	0	0
			699	447	131	119	2			
3	G	79	Total	C	N	O	S	0	0	0
			674	431	125	116	2			
3	H	79	Total	C	N	O	S	0	0	0
			674	431	125	116	2			
3	I	81	Total	C	N	O	S	0	0	0
			688	441	127	118	2			
3	J	83	Total	C	N	O	S	0	0	0
			707	453	132	120	2			
3	K	83	Total	C	N	O	S	0	0	0
			707	453	132	120	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	502	ILE	ASP	ENGINEERED	UNP O15409
G	502	ILE	ASP	ENGINEERED	UNP O15409
H	502	ILE	ASP	ENGINEERED	UNP O15409
I	502	ILE	ASP	ENGINEERED	UNP O15409
J	502	ILE	ASP	ENGINEERED	UNP O15409
K	502	ILE	ASP	ENGINEERED	UNP O15409

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0
4	K	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	I	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	52	Total O 52 52	0	0
5	B	55	Total O 55 55	0	0
5	C	44	Total O 44 44	0	0
5	D	59	Total O 59 59	0	0
5	F	39	Total O 39 39	0	0
5	G	39	Total O 39 39	0	0
5	H	54	Total O 54 54	0	0
5	I	45	Total O 45 45	0	0
5	J	106	Total O 106 106	0	0

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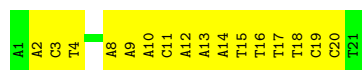
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	K	88	Total	O	0	0
			88	88		

### 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.

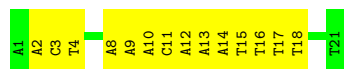
- Molecule 1: 5'-D(\*AP\*AP\*CP\*TP\*AP\*TP\*GP\*AP\*AP\*AP\*CP\*AP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*T)-3'

Chain A: 



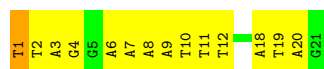
- Molecule 1: 5'-D(\*AP\*AP\*CP\*TP\*AP\*TP\*GP\*AP\*AP\*AP\*CP\*AP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*T)-3'

Chain C: 



- Molecule 2: 5'-D(\*TP\*TP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*TP\*GP\*TP\*TP\*TP\*CP\*AP\*TP\*AP\*G)-3'

Chain B: 



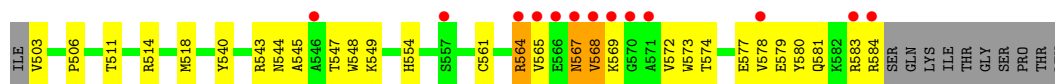
- Molecule 2: 5'-D(\*TP\*TP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*TP\*GP\*TP\*TP\*TP\*CP\*AP\*TP\*AP\*G)-3'

Chain D: 



- Molecule 3: Forkhead box protein P2

Chain F: 



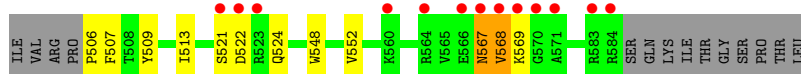
- Molecule 3: Forkhead box protein P2

Chain G: 



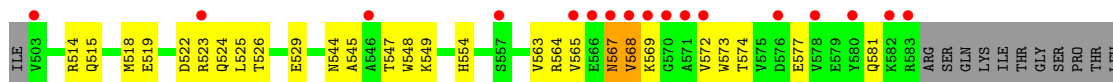
• Molecule 3: Forkhead box protein P2

Chain H:



• Molecule 3: Forkhead box protein P2

Chain I:



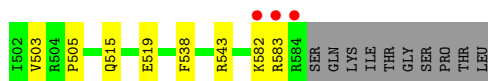
• Molecule 3: Forkhead box protein P2

Chain J:



• Molecule 3: Forkhead box protein P2

Chain K:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.54Å 124.21Å 67.67Å 90.00° 110.81° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 38.38 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.90) 96.3 (38.38-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 1.89Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.222 , 0.244 0.223 , 0.229	Depositor DCC
$R_{free}$ test set	7938 reflections (11.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.4	EDS
Estimated twinning fraction	0.486 for l,-k,h	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	4 of 81612 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% 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	0.40	0/475	0.71	0/730
1	C	0.39	0/475	0.73	0/730
2	B	0.41	0/483	0.75	0/745
2	D	0.38	0/483	0.75	0/745
3	F	0.36	0/717	0.52	0/971
3	G	0.35	0/691	0.55	0/934
3	H	0.35	0/691	0.57	0/934
3	I	0.34	0/706	0.50	0/957
3	J	0.42	0/725	0.60	0/982
3	K	0.42	0/725	0.59	0/982
All	All	0.38	0/6171	0.62	0/8710

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1	DT	Sidechain

## 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	424	0	240	27	0
1	C	424	0	240	24	0
2	B	431	0	242	23	0
2	D	431	0	242	17	0
3	F	699	0	693	31	0
3	G	674	0	665	17	0
3	H	674	0	665	11	0
3	I	688	0	680	21	0
3	J	707	0	704	7	0
3	K	707	0	704	4	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
5	A	52	0	0	0	0
5	B	55	0	0	2	0
5	C	44	0	0	0	0
5	D	59	0	0	1	0
5	F	39	0	0	2	0
5	G	39	0	0	1	0
5	H	54	0	0	1	0
5	I	45	0	0	0	0
5	J	106	0	0	1	0
5	K	88	0	0	1	0
All	All	6446	0	5075	180	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 16.

All (180) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1:DT:H2"	2:B:2:DT:H5"	1.36	1.06

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:568:VAL:HG23	3:G:569:LYS:H	1.34	0.93
3:F:568:VAL:HG13	3:F:569:LYS:H	1.35	0.91
1:A:2:DA:H2''	1:A:3:DC:H5'	1.52	0.91
1:C:12:DA:H2''	1:C:13:DA:H5''	1.55	0.89
3:H:568:VAL:HG23	3:H:569:LYS:H	1.37	0.89
2:B:2:DT:H2''	2:B:3:DA:H5'	1.55	0.88
2:B:2:DT:H2''	2:B:3:DA:C5'	2.03	0.88
1:A:10:DA:H2''	1:A:11:DC:H5'	1.57	0.87
1:A:15:DT:H2''	1:A:16:DT:H5'	1.58	0.86
1:C:2:DA:H2''	1:C:3:DC:H5'	1.56	0.85
2:B:11:DT:H2''	2:B:12:DT:H5'	1.56	0.85
2:D:11:DT:H2''	2:D:12:DT:H5'	1.59	0.82
1:C:15:DT:H2''	1:C:16:DT:H5'	1.62	0.80
1:C:10:DA:H2''	1:C:11:DC:H5'	1.63	0.80
1:C:12:DA:H2''	1:C:13:DA:C5'	2.12	0.79
1:A:12:DA:H2''	1:A:13:DA:C5'	2.13	0.77
1:C:12:DA:C2'	1:C:13:DA:H5''	2.16	0.76
2:D:4:DG:H2''	2:D:5:DG:H5'	1.67	0.76
1:A:12:DA:H2''	1:A:13:DA:H5''	1.68	0.74
1:C:14:DA:H2''	1:C:15:DT:H5''	1.69	0.74
1:A:14:DA:H2''	1:A:15:DT:H5''	1.71	0.73
2:B:11:DT:H2''	2:B:12:DT:C5'	2.19	0.72
1:C:14:DA:H2''	1:C:15:DT:C5'	2.20	0.71
2:D:10:DT:H2''	2:D:11:DT:H5'	1.72	0.71
3:J:580:TYR:O	3:J:584:ARG:HD3	1.91	0.71
2:D:10:DT:H2''	2:D:11:DT:C5'	2.21	0.71
2:D:11:DT:H2''	2:D:12:DT:C5'	2.21	0.70
2:B:10:DT:H2''	2:B:11:DT:C5'	2.21	0.70
1:A:12:DA:C2'	1:A:13:DA:H5''	2.23	0.69
1:A:14:DA:H2''	1:A:15:DT:C5'	2.23	0.68
3:J:582:LYS:O	3:J:583:ARG:HB2	1.92	0.68
3:F:568:VAL:HG13	3:F:569:LYS:N	2.08	0.67
3:I:577:GLU:O	3:I:581:GLN:HG2	1.95	0.67
3:I:568:VAL:HG12	3:I:568:VAL:O	1.93	0.67
1:C:14:DA:C2'	1:C:15:DT:H5''	2.25	0.67
1:C:8:DA:H2''	1:C:9:DA:H5'	1.77	0.66
2:B:2:DT:H2''	2:B:3:DA:H5''	1.76	0.66
3:H:522:ASP:O	3:H:524:GLN:HG3	1.95	0.66
1:A:10:DA:H2''	1:A:11:DC:C5'	2.26	0.66
1:C:10:DA:H2''	1:C:11:DC:C5'	2.25	0.66
2:B:10:DT:H2''	2:B:11:DT:H5'	1.79	0.65
3:K:582:LYS:O	3:K:583:ARG:HB2	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:522:ASP:O	3:I:524:GLN:HG3	1.98	0.64
1:A:14:DA:C2'	1:A:15:DT:H5''	2.27	0.64
1:A:8:DA:H2''	1:A:9:DA:H5'	1.80	0.62
3:G:522:ASP:O	3:G:524:GLN:HG3	2.00	0.62
3:I:565:VAL:O	3:I:572:VAL:HG22	2.00	0.62
1:C:15:DT:H2''	1:C:16:DT:C5'	2.30	0.62
3:F:564:ARG:H	3:F:564:ARG:HD3	1.66	0.61
2:D:2:DT:H2''	2:D:3:DA:H5'	1.83	0.59
3:F:578:VAL:O	3:F:581:GLN:HB3	2.02	0.59
1:C:17:DT:H2''	1:C:18:DT:H5'	1.85	0.59
3:I:526:THR:OG1	3:I:529:GLU:HG3	2.02	0.59
2:D:3:DA:H2''	2:D:4:DG:O5'	2.03	0.58
1:A:12:DA:H2''	1:A:13:DA:H5'	1.87	0.57
2:B:19:DT:H2''	2:B:20:DA:N7	2.19	0.57
1:A:17:DT:H2''	1:A:18:DT:C5'	2.35	0.56
3:K:503:VAL:HG13	5:K:665:HOH:O	2.06	0.56
3:G:506:PRO:HG2	3:G:507:PHE:H	1.70	0.56
3:I:567:ASN:HD22	3:I:567:ASN:H	1.53	0.56
2:B:1:DT:C2'	2:B:2:DT:H5''	2.23	0.56
1:C:17:DT:H2''	1:C:18:DT:C5'	2.36	0.56
1:A:15:DT:H2''	1:A:16:DT:C5'	2.32	0.55
2:B:8:DA:H2''	2:B:9:DA:C5'	2.36	0.55
5:B:26:HOH:O	3:F:554:HIS:HE1	1.89	0.54
3:G:568:VAL:HG23	3:G:569:LYS:N	2.14	0.54
3:F:567:ASN:H	3:F:567:ASN:HD22	1.55	0.54
5:B:58:HOH:O	3:F:547:THR:HG22	2.07	0.54
3:I:545:ALA:HA	3:I:548:TRP:NE1	2.22	0.54
3:J:503:VAL:HG13	5:J:671:HOH:O	2.06	0.54
3:F:565:VAL:HG13	3:F:565:VAL:O	2.08	0.54
3:J:507:PHE:HB2	3:J:512:LEU:HD13	1.90	0.53
3:F:545:ALA:O	3:F:549:LYS:HB2	2.09	0.53
2:D:1:DT:H2''	2:D:2:DT:OP2	2.08	0.53
3:F:503:VAL:HG12	3:F:503:VAL:O	2.09	0.53
3:I:545:ALA:O	3:I:549:LYS:HB2	2.09	0.52
3:F:514:ARG:CZ	3:F:518:MET:SD	2.97	0.52
3:H:521:SER:O	3:H:522:ASP:HB2	2.09	0.52
3:I:544:ASN:OD1	3:I:547:THR:N	2.42	0.52
2:D:8:DA:H2''	2:D:9:DA:C5'	2.38	0.52
1:C:8:DA:H2''	1:C:9:DA:C5'	2.40	0.52
3:F:564:ARG:HG2	3:F:564:ARG:O	2.10	0.52
3:F:573:TRP:O	3:F:574:THR:HB	2.10	0.52
3:H:568:VAL:HG23	3:H:569:LYS:N	2.16	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:545:ALA:HA	3:F:548:TRP:NE1	2.24	0.51
2:B:10:DT:H2''	2:B:11:DT:H5''	1.91	0.51
3:F:580:TYR:OH	3:G:511:THR:HA	2.10	0.51
2:B:18:DA:H2''	2:B:19:DT:H5'	1.92	0.51
3:G:564:ARG:HE	3:G:571:ALA:CB	2.24	0.50
2:B:18:DA:H1'	2:B:19:DT:H5''	1.93	0.50
3:F:577:GLU:HG3	3:F:584:ARG:NH2	2.27	0.50
5:D:26:HOH:O	3:I:554:HIS:HE1	1.93	0.50
2:B:19:DT:H2''	2:B:20:DA:C8	2.47	0.50
2:B:10:DT:C2'	2:B:11:DT:H5''	2.41	0.50
3:G:509:TYR:O	3:G:513:ILE:HG13	2.10	0.50
3:F:583:ARG:HG3	5:F:637:HOH:O	2.11	0.50
3:K:505:PRO:HG3	3:K:538:PHE:CD2	2.46	0.50
3:G:550:ASN:OD1	3:G:553:ARG:NH2	2.45	0.49
3:I:563:VAL:O	3:I:574:THR:HG22	2.12	0.49
3:H:567:ASN:HD22	3:H:567:ASN:H	1.61	0.49
3:F:568:VAL:HG22	3:F:569:LYS:N	2.28	0.49
1:A:17:DT:H2''	1:A:18:DT:H5'	1.95	0.49
2:B:8:DA:H2''	2:B:9:DA:H5''	1.95	0.49
3:H:567:ASN:ND2	3:H:567:ASN:H	2.11	0.49
3:F:567:ASN:H	3:F:567:ASN:ND2	2.11	0.48
5:H:374:HOH:O	3:I:547:THR:HG22	2.12	0.48
2:D:8:DA:H2''	2:D:9:DA:H5''	1.95	0.48
2:D:1:DT:H2''	2:D:2:DT:C7	2.44	0.48
1:C:15:DT:H2'	1:C:16:DT:H71	1.96	0.47
2:D:1:DT:C2'	2:D:2:DT:H72	2.43	0.47
1:A:8:DA:H2''	1:A:9:DA:C5'	2.42	0.47
3:F:581:GLN:HA	3:F:584:ARG:HG3	1.96	0.47
3:I:567:ASN:ND2	3:I:567:ASN:H	2.13	0.47
3:H:509:TYR:O	3:H:513:ILE:HG13	2.14	0.47
3:F:567:ASN:N	3:F:567:ASN:HD22	2.11	0.47
3:I:515:GLN:O	3:I:519:GLU:HG3	2.14	0.47
3:J:505:PRO:HG3	3:J:538:PHE:CD2	2.48	0.47
1:C:3:DC:H2''	1:C:4:DT:OP2	2.15	0.47
2:B:10:DT:H1'	2:B:11:DT:H5''	1.96	0.47
2:D:10:DT:H1'	2:D:11:DT:H5''	1.97	0.47
2:D:10:DT:C2'	2:D:11:DT:H5''	2.45	0.47
3:I:518:MET:SD	3:I:523:ARG:NH1	2.88	0.47
3:F:564:ARG:N	3:F:564:ARG:HD3	2.29	0.46
2:D:10:DT:H2''	2:D:11:DT:H5''	1.97	0.46
3:I:526:THR:HG23	3:I:529:GLU:OE2	2.15	0.46
3:F:564:ARG:H	3:F:564:ARG:CD	2.28	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:526:THR:OG1	3:G:529:GLU:HG3	2.16	0.46
3:G:567:ASN:ND2	3:G:567:ASN:H	2.14	0.46
1:A:3:DC:H2''	1:A:4:DT:OP2	2.15	0.45
1:A:13:DA:H2''	1:A:14:DA:C8	2.51	0.45
3:G:567:ASN:HD22	3:G:567:ASN:H	1.63	0.45
3:G:579:GLU:OE1	3:G:579:GLU:HA	2.16	0.45
2:B:3:DA:H2''	2:B:4:DG:O5'	2.16	0.45
3:I:524:GLN:O	3:I:525:LEU:HD23	2.16	0.45
3:F:506:PRO:HD2	5:F:606:HOH:O	2.15	0.45
3:I:564:ARG:HD3	3:I:573:TRP:CH2	2.52	0.45
1:C:13:DA:H2''	1:C:14:DA:C8	2.52	0.45
1:A:12:DA:H1'	1:A:13:DA:H5''	1.99	0.45
3:H:567:ASN:N	3:H:567:ASN:HD22	2.13	0.45
3:G:567:ASN:HD22	3:G:567:ASN:N	2.14	0.45
3:F:581:GLN:HA	3:F:584:ARG:CD	2.47	0.44
3:I:514:ARG:O	3:I:518:MET:HG2	2.17	0.44
2:B:8:DA:C2'	2:B:9:DA:H5''	2.48	0.44
3:H:521:SER:O	3:H:522:ASP:CB	2.65	0.44
1:C:14:DA:H1'	1:C:15:DT:H5''	1.99	0.44
1:A:15:DT:C6	1:A:16:DT:H72	2.53	0.44
3:H:506:PRO:HG2	3:H:507:PHE:H	1.83	0.44
1:A:17:DT:H2''	1:A:18:DT:H5''	2.00	0.44
2:D:8:DA:C2'	2:D:9:DA:H5''	2.48	0.44
3:F:511:THR:HG22	3:G:584:ARG:NH2	2.32	0.44
3:G:521:SER:O	3:G:522:ASP:HB2	2.18	0.44
1:A:14:DA:H1'	1:A:15:DT:H5''	1.99	0.43
3:F:540:TYR:O	3:F:543:ARG:HD2	2.19	0.43
1:A:14:DA:H2''	1:A:15:DT:H5'	2.00	0.43
3:F:565:VAL:HG13	3:F:572:VAL:HG23	2.00	0.43
3:K:515:GLN:O	3:K:519:GLU:HG3	2.19	0.43
1:A:8:DA:H1'	1:A:9:DA:H5''	2.01	0.43
3:I:567:ASN:HD22	3:I:567:ASN:N	2.10	0.43
1:A:19:DC:H1'	1:A:20:DC:H5''	2.00	0.43
2:B:2:DT:C2'	2:B:3:DA:H5''	2.46	0.43
2:B:8:DA:H2''	2:B:9:DA:H5'	2.00	0.43
3:J:583:ARG:HA	3:J:583:ARG:HD3	1.91	0.43
1:C:8:DA:H1'	1:C:9:DA:H5''	2.01	0.42
3:G:526:THR:HG1	3:G:529:GLU:HG3	1.83	0.42
2:D:1:DT:H2''	2:D:2:DT:H72	2.01	0.42
3:F:564:ARG:CG	3:F:564:ARG:O	2.67	0.42
3:I:567:ASN:HD21	3:I:569:LYS:HB2	1.85	0.42
3:F:544:ASN:OD1	3:F:547:THR:N	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:14:DA:H2''	1:C:15:DT:H5'	1.97	0.42
1:C:10:DA:C2'	1:C:11:DC:C5'	2.97	0.41
1:C:12:DA:H2''	1:C:13:DA:H5'	1.95	0.41
3:G:560:LYS:HG3	5:G:619:HOH:O	2.20	0.41
3:F:561:CYS:HA	3:F:579:GLU:HB3	2.03	0.41
3:H:548:TRP:O	3:H:552:VAL:HG23	2.20	0.41
1:A:3:DC:C6	1:A:4:DT:H72	2.56	0.41
1:A:10:DA:C2'	1:A:11:DC:C5'	2.98	0.41
1:C:3:DC:C6	1:C:4:DT:H72	2.56	0.41
2:B:6:DA:H2''	2:B:7:DA:C5'	2.51	0.41
3:J:525:LEU:HD22	3:J:529:GLU:HB3	2.02	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	
3	F	80/93 (86%)	75 (94%)	4 (5%)	1 (1%)	18	5
3	G	77/93 (83%)	75 (97%)	1 (1%)	1 (1%)	18	5
3	H	77/93 (83%)	72 (94%)	4 (5%)	1 (1%)	18	5
3	I	79/93 (85%)	73 (92%)	5 (6%)	1 (1%)	18	5
3	J	81/93 (87%)	79 (98%)	2 (2%)	0	100	100
3	K	81/93 (87%)	80 (99%)	1 (1%)	0	100	100
All	All	475/558 (85%)	454 (96%)	17 (4%)	4 (1%)	27	12

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	568	VAL
3	G	568	VAL
3	H	568	VAL
3	I	568	VAL



### 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	
3	F	74/84 (88%)	72 (97%)	2 (3%)	57	47
3	G	71/84 (84%)	70 (99%)	1 (1%)	78	75
3	H	71/84 (84%)	70 (99%)	1 (1%)	78	75
3	I	73/84 (87%)	72 (99%)	1 (1%)	78	75
3	J	75/84 (89%)	73 (97%)	2 (3%)	57	47
3	K	75/84 (89%)	74 (99%)	1 (1%)	80	77
All	All	439/504 (87%)	431 (98%)	8 (2%)	71	66

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	564	ARG
3	F	567	ASN
3	G	567	ASN
3	H	567	ASN
3	I	567	ASN
3	J	512	LEU
3	J	543	ARG
3	K	543	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	554	HIS
3	F	567	ASN
3	G	524	GLN
3	G	544	ASN
3	G	567	ASN
3	H	515	GLN
3	H	544	ASN
3	H	567	ASN
3	I	554	HIS
3	I	567	ASN

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Mol	Chain	Res	Type
3	J	528	ASN
3	J	555	ASN
3	K	524	GLN
3	K	528	ASN
3	K	555	ASN

### 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 6 ligands modelled in this entry, 6 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	21/21 (100%)	0.02	0 100 100	13, 32, 64, 65	0
1	C	21/21 (100%)	-0.05	0 100 100	14, 32, 62, 64	0
2	B	21/21 (100%)	-0.04	0 100 100	17, 23, 62, 72	0
2	D	21/21 (100%)	-0.15	0 100 100	17, 23, 59, 67	0
3	F	82/93 (88%)	0.77	13 (15%) 3 2	18, 41, 74, 89	0
3	G	79/93 (84%)	0.42	9 (11%) 6 5	17, 31, 72, 82	0
3	H	79/93 (84%)	0.92	13 (16%) 2 2	17, 33, 100, 111	0
3	I	81/93 (87%)	1.24	17 (20%) 1 1	18, 49, 104, 111	0
3	J	83/93 (89%)	-0.24	2 (2%) 56 57	12, 20, 43, 80	0
3	K	83/93 (89%)	-0.13	3 (3%) 41 42	11, 20, 52, 104	0
All	All	571/642 (88%)	0.41	57 (9%) 7 7	11, 30, 85, 111	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	568	VAL	15.9
3	I	570	GLY	11.9
3	I	568	VAL	9.0
3	K	583	ARG	8.8
3	H	567	ASN	8.8
3	H	569	LYS	8.8
3	H	570	GLY	8.0
3	I	569	LYS	7.4
3	F	570	GLY	6.9
3	I	566	GLU	6.9
3	G	568	VAL	6.8
3	F	568	VAL	6.4
3	I	571	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
3	G	570	GLY	5.8
3	I	578	VAL	5.7
3	H	522	ASP	5.3
3	H	566	GLU	5.1
3	I	583	ARG	4.5
3	J	583	ARG	4.3
3	G	569	LYS	4.3
3	K	584	ARG	4.3
3	H	521	SER	4.0
3	I	565	VAL	3.9
3	I	567	ASN	3.8
3	G	521	SER	3.8
3	F	583	ARG	3.7
3	G	522	ASP	3.6
3	F	569	LYS	3.5
3	F	571	ALA	3.4
3	H	584	ARG	3.0
3	G	567	ASN	3.0
3	I	503	VAL	3.0
3	H	523	ARG	3.0
3	I	557	SER	2.9
3	F	546	ALA	2.9
3	K	582	LYS	2.8
3	I	546	ALA	2.8
3	I	580	TYR	2.8
3	H	571	ALA	2.8
3	F	564	ARG	2.7
3	F	557	SER	2.7
3	F	567	ASN	2.7
3	H	583	ARG	2.6
3	I	576	ASP	2.5
3	H	564	ARG	2.5
3	F	565	VAL	2.5
3	G	566	GLU	2.5
3	G	523	ARG	2.5
3	F	566	GLU	2.5
3	I	523	ARG	2.3
3	F	584	ARG	2.2
3	I	572	VAL	2.2
3	I	582	LYS	2.2
3	F	578	VAL	2.1
3	H	560	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	J	584	ARG	2.1
3	G	560	LYS	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(Å <sup>2</sup> )	Q<0.9
4	MG	I	603	1/1	0.34	2.11	82,82,82,82	0
4	MG	F	601	1/1	0.19	0.16	69,69,69,69	0
4	MG	H	602	1/1	0.13	-0.05	38,38,38,38	0
4	MG	G	604	1/1	0.08	-0.56	34,34,34,34	0
4	MG	J	605	1/1	0.06	-1.10	18,18,18,18	0
4	MG	K	606	1/1	0.04	-1.71	21,21,21,21	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.