



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:31 pm BST

PDB ID : 1MDM  
Title : INHIBITED FRAGMENT OF ETS-1 AND PAIRED DOMAIN OF PAX5  
BOUND TO DNA  
Authors : Garvie, C.W.; Pufall, M.A.; Graves, B.J.; Wolberger, C.  
Deposited on : 2002-08-07  
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](mailto: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 ⓘ 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  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

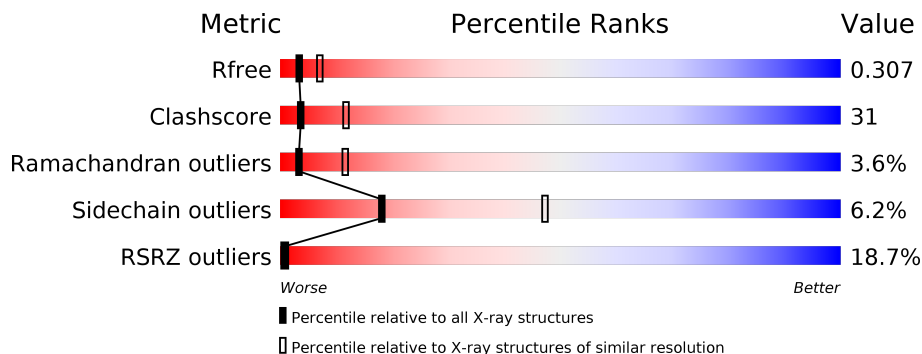
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	C	26	 4% (poor fit), 35% (0 outliers), 62% (1 outlier), 0% (2 outliers), 0% (3+ outliers)
2	D	26	 8% (poor fit), 54% (0 outliers), 42% (1 outlier), 0% (2 outliers), 0% (3+ outliers)
3	A	149	 30% (poor fit), 42% (0 outliers), 39% (1 outlier), 17% (2 outliers), 0% (3+ outliers)
4	B	161	 6% (poor fit), 33% (0 outliers), 40% (1 outlier), 0% (2 outliers), 20% (3+ outliers)

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3054 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 DNA chain called PAX5/ETS BINDING SITE ON THE MB-1 PROMOTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	26	533	253	98	157	25	0	0	0

- Molecule 2 is a DNA chain called PAX5/ETS BINDING SITE ON THE MB-1 PROMOTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	D	26	527	250	101	151	25	0	0	0

- Molecule 3 is a protein called PAIRED BOX PROTEIN PAX-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	124	964	604	186	170	4	0	0	0

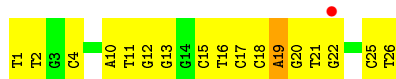
- Molecule 4 is a protein called C-ETS-1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	129	1030	664	178	184	4	0	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

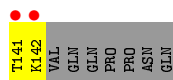
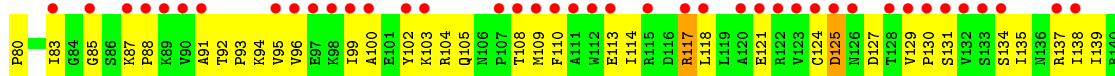
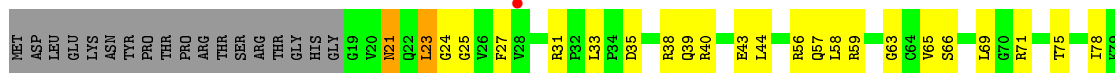
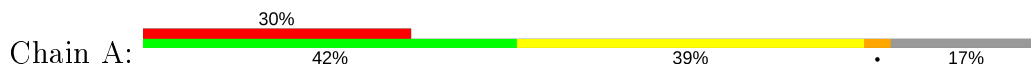
- Molecule 1: PAX5/ETS BINDING SITE ON THE MB-1 PROMOTER



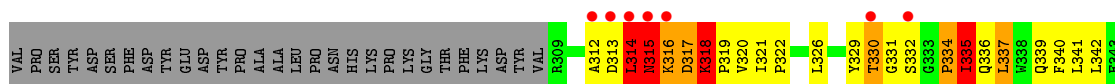
- Molecule 2: PAX5/ETS BINDING SITE ON THE MB-1 PROMOTER

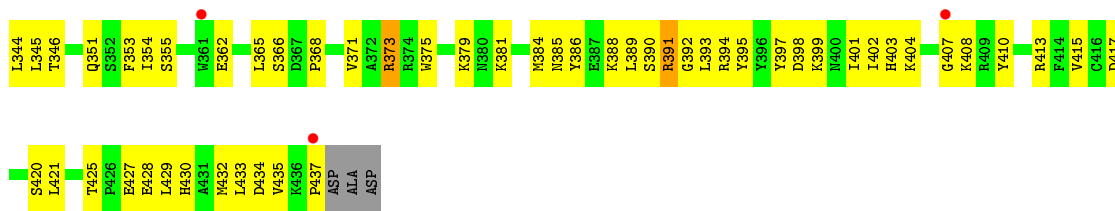


- Molecule 3: PAIRED BOX PROTEIN PAX-5



- Molecule 4: C-ETS-1 PROTEIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.27Å 171.23Å 44.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.03 – 2.80 39.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.3 (32.03-2.80) 87.4 (39.63-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 2.81Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.259 , 0.310 0.260 , 0.307	Depositor DCC
$R_{free}$ test set	1373 reflections (10.27%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.7	Xtrriage
Anisotropy	0.382	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 62.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	3054	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.66% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	C	0.56	0/597	0.74	0/921
2	D	0.52	0/591	0.72	0/909
3	A	0.37	0/980	0.63	0/1324
4	B	0.75	1/1057 (0.1%)	0.85	6/1431 (0.4%)
All	All	0.58	1/3225 (0.0%)	0.75	6/4585 (0.1%)

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	C	0	1
2	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	334	PRO	N-CD	-18.10	1.22	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	316	LYS	N-CA-C	8.22	133.19	111.00
4	B	317	ASP	N-CA-C	6.65	128.97	111.00
4	B	315	ASN	C-N-CA	5.81	136.23	121.70
4	B	334	PRO	N-CD-CG	5.52	111.49	103.20
4	B	318	LYS	N-CA-C	5.42	125.63	111.00
4	B	437	PRO	N-CA-CB	5.17	109.50	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	19	DA	Sidechain
2	D	14	DC	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	C	533	0	294	25	0
2	D	527	0	291	13	0
3	A	964	0	1007	69	0
4	B	1030	0	1000	77	0
All	All	3054	0	2592	172	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 31.

All (172) 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)
4:B:425:THR:OG1	4:B:428:GLU:HG3	1.29	1.30
4:B:330:THR:CG2	4:B:421:LEU:HD11	1.70	1.20
4:B:330:THR:HG22	4:B:421:LEU:HD11	1.23	1.19
4:B:326:LEU:HD11	4:B:330:THR:CG2	1.79	1.12
4:B:330:THR:HG22	4:B:421:LEU:CD1	1.87	1.04
4:B:319:PRO:HG2	4:B:322:PRO:HG3	1.41	1.02
4:B:326:LEU:HD11	4:B:330:THR:HG23	1.45	0.97
3:A:21:ASN:HD21	3:A:25:GLY:H	1.13	0.94
4:B:326:LEU:CD1	4:B:330:THR:HG23	2.00	0.91
4:B:425:THR:OG1	4:B:428:GLU:CG	2.16	0.91
4:B:330:THR:CG2	4:B:421:LEU:CD1	2.48	0.89
4:B:401:ILE:HG22	4:B:402:ILE:HG12	1.57	0.86
4:B:326:LEU:HD11	4:B:330:THR:HG21	1.54	0.86
1:C:12:DG:H4'	1:C:13:DG:OP1	1.77	0.84
4:B:313:ASP:O	4:B:315:ASN:N	2.13	0.81
3:A:21:ASN:HD22	3:A:21:ASN:C	1.86	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:DC:H6	1:C:17:DC:H5'	1.48	0.79
3:A:40:ARG:NH1	3:A:43:GLU:HG2	1.99	0.78
4:B:368:PRO:HG3	4:B:410:TYR:CE2	2.20	0.77
4:B:365:LEU:O	4:B:368:PRO:HD3	1.87	0.74
1:C:19:DA:H1'	1:C:20:DG:H5'	1.70	0.74
4:B:330:THR:HG21	4:B:421:LEU:HD11	1.70	0.73
4:B:391:ARG:HH11	4:B:391:ARG:HG3	1.54	0.71
4:B:326:LEU:CD1	4:B:330:THR:CG2	2.61	0.71
2:D:1:DA:H2''	2:D:2:DA:C8	2.26	0.71
4:B:407:GLY:O	4:B:408:LYS:HG3	1.92	0.69
3:A:21:ASN:HD21	3:A:25:GLY:N	1.88	0.69
2:D:9:DT:H2''	2:D:10:DG:C8	2.29	0.67
2:D:14:DC:H2''	2:D:15:DC:C6	2.31	0.66
3:A:95:VAL:O	3:A:99:ILE:HG12	1.95	0.65
3:A:94:LYS:HG3	3:A:95:VAL:N	2.11	0.65
3:A:92:THR:HG23	3:A:93:PRO:HD2	1.79	0.65
3:A:21:ASN:ND2	3:A:25:GLY:H	1.89	0.64
3:A:38:ARG:NH2	3:A:80:PRO:HB3	2.12	0.64
4:B:320:VAL:HB	4:B:346:THR:HB	1.79	0.64
4:B:353:PHE:HA	4:B:366:SER:HB2	1.80	0.64
4:B:365:LEU:HD22	4:B:371:VAL:HG21	1.81	0.63
3:A:117:ARG:O	3:A:121:GLU:HG3	1.98	0.63
3:A:33:LEU:O	3:A:38:ARG:HD2	1.99	0.63
1:C:16:DT:H2''	1:C:17:DC:C5'	2.29	0.62
3:A:102:TYR:HD1	3:A:114:ILE:HG23	1.64	0.62
3:A:99:ILE:HD11	3:A:118:LEU:HD11	1.81	0.62
4:B:318:LYS:CB	4:B:319:PRO:CD	2.77	0.62
1:C:16:DT:H2''	1:C:17:DC:H5'	1.80	0.62
3:A:87:LYS:HE2	3:A:88:PRO:HD3	1.82	0.61
4:B:391:ARG:HG3	4:B:391:ARG:NH1	2.14	0.61
4:B:429:LEU:HA	4:B:432:MET:HE3	1.83	0.60
2:D:12:DA:H2''	2:D:13:DG:C8	2.37	0.60
3:A:141:THR:O	3:A:142:LYS:HG3	2.02	0.60
3:A:63:GLY:O	3:A:66:SER:HB3	2.02	0.60
3:A:40:ARG:HH12	3:A:43:GLU:HG2	1.67	0.60
4:B:425:THR:HG1	4:B:428:GLU:HG3	1.61	0.60
1:C:17:DC:C6	1:C:17:DC:H5'	2.34	0.59
4:B:427:GLU:CD	4:B:427:GLU:H	2.05	0.59
1:C:21:DT:H72	3:A:137:ARG:HD2	1.83	0.59
4:B:403:HIS:HD2	4:B:415:VAL:HG11	1.68	0.58
4:B:330:THR:HG21	4:B:421:LEU:CG	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:DT:H2'	3:A:137:ARG:HH21	1.69	0.57
3:A:96:VAL:CG1	3:A:142:LYS:HD3	2.33	0.57
4:B:318:LYS:CB	4:B:319:PRO:HD3	2.35	0.57
3:A:109:MET:SD	3:A:114:ILE:HD13	2.44	0.57
3:A:134:SER:O	3:A:138:ILE:HG12	2.05	0.57
1:C:1:DT:H2''	1:C:2:DT:OP2	2.05	0.56
3:A:21:ASN:ND2	3:A:24:GLY:H	2.04	0.56
4:B:429:LEU:HA	4:B:432:MET:CE	2.35	0.56
4:B:321:ILE:HG22	4:B:321:ILE:O	2.05	0.56
4:B:334:PRO:O	4:B:335:ILE:HG22	2.05	0.56
3:A:92:THR:HG21	3:A:94:LYS:NZ	2.20	0.55
4:B:329:TYR:CD2	4:B:330:THR:HG23	2.41	0.55
3:A:96:VAL:HG13	3:A:142:LYS:HD3	1.89	0.55
3:A:21:ASN:ND2	3:A:25:GLY:N	2.51	0.55
4:B:429:LEU:HD12	4:B:432:MET:CE	2.37	0.55
4:B:384:MET:HG3	4:B:385:ASN:N	2.22	0.55
4:B:403:HIS:CD2	4:B:415:VAL:HG11	2.42	0.54
3:A:131:SER:O	3:A:135:ILE:HG13	2.07	0.54
4:B:375:TRP:CD1	4:B:389:LEU:HD23	2.43	0.54
4:B:319:PRO:O	4:B:322:PRO:HD3	2.07	0.54
3:A:134:SER:O	3:A:137:ARG:HB3	2.08	0.54
3:A:21:ASN:C	3:A:21:ASN:ND2	2.58	0.53
1:C:4:DC:H5''	4:B:404:LYS:NZ	2.22	0.53
3:A:87:LYS:HE2	3:A:88:PRO:CD	2.37	0.53
3:A:23:LEU:CD1	4:B:399:LYS:HE3	2.38	0.53
3:A:135:ILE:O	3:A:139:ILE:HG12	2.08	0.53
1:C:19:DA:H2''	1:C:20:DG:O5'	2.08	0.52
1:C:4:DC:H5''	4:B:404:LYS:HZ3	1.73	0.52
4:B:331:GLY:O	4:B:332:SER:OG	2.26	0.52
2:D:1:DA:N3	2:D:1:DA:H2'	2.24	0.51
4:B:337:LEU:HD22	4:B:337:LEU:O	2.10	0.51
1:C:21:DT:H2'	3:A:137:ARG:NH2	2.25	0.51
3:A:92:THR:O	3:A:96:VAL:HG23	2.10	0.51
4:B:394:ARG:HA	4:B:397:TYR:CE1	2.47	0.50
4:B:417:ASP:OD1	4:B:420:SER:N	2.39	0.50
3:A:125:ASP:C	3:A:127:ASP:H	2.15	0.50
3:A:65:VAL:HG12	3:A:69:LEU:CD1	2.42	0.49
2:D:6:DC:H2''	2:D:7:DA:N7	2.26	0.49
4:B:330:THR:HG21	4:B:421:LEU:CD1	2.32	0.49
3:A:103:LYS:HG3	3:A:139:ILE:HD12	1.94	0.49
3:A:71:ARG:O	3:A:75:THR:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:94:LYS:HG3	3:A:95:VAL:H	1.78	0.49
4:B:346:THR:HA	4:B:433:LEU:HD11	1.93	0.49
3:A:92:THR:CG2	3:A:93:PRO:HD2	2.41	0.49
2:D:14:DC:H2''	2:D:15:DC:C5	2.48	0.49
4:B:362:GLU:HB2	4:B:413:ARG:CZ	2.43	0.48
4:B:391:ARG:O	4:B:391:ARG:HG3	2.14	0.48
1:C:21:DT:H72	3:A:137:ARG:CD	2.44	0.48
3:A:56:ARG:HD2	4:B:398:ASP:OD2	2.13	0.48
2:D:10:DG:H2''	2:D:11:DG:C8	2.49	0.48
4:B:373:ARG:HB2	4:B:373:ARG:CZ	2.44	0.48
4:B:345:LEU:O	4:B:433:LEU:HD13	2.14	0.48
4:B:425:THR:CB	4:B:428:GLU:HG3	2.35	0.48
3:A:39:GLN:OE1	3:A:78:ILE:HD13	2.14	0.47
4:B:326:LEU:HD12	4:B:330:THR:HG23	1.89	0.47
4:B:365:LEU:HB2	4:B:410:TYR:HB3	1.96	0.47
4:B:313:ASP:O	4:B:314:LEU:C	2.52	0.47
4:B:429:LEU:HD12	4:B:432:MET:HE3	1.97	0.46
2:D:12:DA:H2''	2:D:13:DG:H8	1.80	0.46
3:A:31:ARG:HH21	3:A:83:ILE:HD12	1.81	0.46
1:C:10:DA:H2''	1:C:11:DT:H5'	1.97	0.46
3:A:23:LEU:HD13	4:B:399:LYS:HE3	1.97	0.46
4:B:403:HIS:CD2	4:B:415:VAL:HG21	2.51	0.46
4:B:329:TYR:HD2	4:B:330:THR:HG23	1.81	0.46
1:C:15:DC:C2'	1:C:16:DT:H72	2.45	0.46
3:A:87:LYS:HA	3:A:87:LYS:HE2	1.97	0.46
3:A:94:LYS:CG	3:A:95:VAL:N	2.78	0.45
1:C:10:DA:H1'	1:C:11:DT:H5''	1.99	0.45
4:B:335:ILE:CG2	4:B:335:ILE:O	2.65	0.45
4:B:353:PHE:CA	4:B:366:SER:HB2	2.46	0.45
4:B:336:GLN:O	4:B:339:GLN:N	2.50	0.45
3:A:141:THR:O	3:A:142:LYS:CG	2.63	0.45
4:B:384:MET:CG	4:B:385:ASN:N	2.80	0.45
1:C:16:DT:H1'	1:C:17:DC:H5''	1.98	0.45
3:A:130:PRO:O	3:A:135:ILE:HD11	2.16	0.45
3:A:100:ALA:O	3:A:104:ARG:HB2	2.17	0.44
3:A:57:GLN:C	3:A:59:ARG:H	2.20	0.44
1:C:18:DC:H2''	1:C:19:DA:N7	2.31	0.44
3:A:138:ILE:O	3:A:142:LYS:HB2	2.18	0.44
4:B:337:LEU:HD22	4:B:337:LEU:C	2.38	0.44
3:A:92:THR:HG21	3:A:94:LYS:HZ2	1.80	0.44
4:B:330:THR:CB	4:B:421:LEU:HD11	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:110:PHE:O	3:A:114:ILE:HG12	2.18	0.43
4:B:340:PHE:CE2	4:B:344:LEU:HD11	2.53	0.43
3:A:130:PRO:HB2	3:A:135:ILE:HG12	2.01	0.43
4:B:386:TYR:O	4:B:390:SER:OG	2.34	0.43
1:C:21:DT:H2''	1:C:22:DG:C8	2.54	0.43
2:D:16:DC:H5''	3:A:27:PHE:CD2	2.54	0.43
3:A:40:ARG:HA	3:A:40:ARG:HD2	1.76	0.43
2:D:1:DA:H2''	2:D:2:DA:N7	2.33	0.43
3:A:141:THR:O	3:A:141:THR:HG22	2.19	0.42
3:A:110:PHE:HB2	3:A:113:GLU:HG3	2.01	0.42
3:A:105:GLN:CD	3:A:117:ARG:HH22	2.21	0.42
3:A:71:ARG:HH11	3:A:71:ARG:HG2	1.84	0.42
3:A:124:CYS:HB3	3:A:129:VAL:N	2.35	0.42
4:B:392:GLY:O	4:B:395:TYR:HB3	2.18	0.42
1:C:25:DC:H2''	1:C:26:DT:C6	2.55	0.42
4:B:354:ILE:HG12	4:B:355:SER:N	2.35	0.42
4:B:379:LYS:O	4:B:381:LYS:HG2	2.19	0.42
3:A:102:TYR:N	3:A:102:TYR:CD2	2.88	0.41
1:C:22:DG:H2'	3:A:131:SER:OG	2.21	0.41
4:B:373:ARG:HB2	4:B:373:ARG:NH1	2.36	0.41
3:A:38:ARG:NH2	3:A:71:ARG:NH2	2.68	0.41
4:B:341:LEU:HD11	4:B:393:LEU:HD21	2.02	0.41
4:B:430:HIS:HA	4:B:435:VAL:HG21	2.02	0.41
3:A:129:VAL:HA	3:A:130:PRO:HD3	1.87	0.41
2:D:6:DC:H1'	2:D:7:DA:N7	2.36	0.41
3:A:21:ASN:ND2	3:A:24:GLY:N	2.69	0.41
2:D:10:DG:N2	3:A:85:GLY:O	2.54	0.41
4:B:312:ALA:C	4:B:314:LEU:H	2.24	0.41
4:B:385:ASN:ND2	4:B:388:LYS:HE2	2.36	0.40
1:C:15:DC:H2'	1:C:16:DT:H72	2.03	0.40
1:C:1:DT:H2''	1:C:2:DT:H72	2.04	0.40
3:A:44:LEU:HD11	3:A:58:LEU:HD11	2.02	0.40
1:C:12:DG:H2'	1:C:12:DG:O5'	2.21	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	
3	A	122/149 (82%)	110 (90%)	11 (9%)	1 (1%)	19	49
4	B	127/161 (79%)	98 (77%)	21 (16%)	8 (6%)	1	3
All	All	249/310 (80%)	208 (84%)	32 (13%)	9 (4%)	3	11

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	315	ASN
4	B	316	LYS
4	B	317	ASP
4	B	318	LYS
4	B	351	GLN
4	B	314	LEU
4	B	330	THR
4	B	335	ILE
3	A	91	ALA

### 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	
3	A	107/131 (82%)	101 (94%)	6 (6%)	21	51
4	B	104/140 (74%)	97 (93%)	7 (7%)	16	43
All	All	211/271 (78%)	198 (94%)	13 (6%)	18	47

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	21	ASN
3	A	23	LEU
3	A	35	ASP
3	A	108	THR
3	A	117	ARG
3	A	125	ASP
4	B	314	LEU
4	B	335	ILE
4	B	337	LEU
4	B	342	LEU
4	B	373	ARG
4	B	391	ARG
4	B	434	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	21	ASN
3	A	136	ASN
4	B	351	GLN
4	B	380	ASN
4	B	403	HIS
4	B	419	GLN

### 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](#)

There are no ligands in this entry.

## 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	C	26/26 (100%)	0.39	1 (3%) 40 30	29, 54, 105, 124	0
2	D	26/26 (100%)	0.54	2 (7%) 13 7	26, 58, 124, 128	0
3	A	124/149 (83%)	1.94	44 (35%) 0 0	19, 74, 194, 200	0
4	B	129/161 (80%)	0.33	10 (7%) 13 7	17, 51, 112, 137	0
All	All	305/362 (84%)	1.01	57 (18%) 1 1	17, 57, 182, 200	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	99	ILE	16.2
3	A	126	ASN	10.4
3	A	108	THR	9.9
3	A	124	CYS	8.3
3	A	118	LEU	7.9
3	A	141	THR	7.5
3	A	123	VAL	7.2
3	A	120	ALA	7.2
3	A	107	PRO	7.0
3	A	89	LYS	6.6
4	B	315	ASN	6.6
3	A	100	ALA	6.3
3	A	132	VAL	5.9
4	B	330	THR	5.9
3	A	96	VAL	5.7
4	B	312	ALA	5.7
3	A	103	LYS	5.2
3	A	95	VAL	5.2
3	A	133	SER	5.2
3	A	130	PRO	4.6
3	A	109	MET	4.6

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Mol	Chain	Res	Type	RSRZ
3	A	97	GLU	4.5
3	A	121	GLU	4.5
3	A	134	SER	4.5
3	A	117	ARG	4.3
4	B	437	PRO	4.2
3	A	115	ARG	4.1
3	A	110	PHE	4.1
3	A	111	ALA	3.9
3	A	112	TRP	3.9
3	A	102	TYR	3.7
3	A	90	VAL	3.6
3	A	125	ASP	3.3
3	A	85	GLY	3.3
3	A	138	ILE	3.2
3	A	142	LYS	3.2
4	B	332	SER	2.8
3	A	131	SER	2.6
3	A	137	ARG	2.6
3	A	113	GLU	2.5
4	B	407	GLY	2.5
3	A	87	LYS	2.4
3	A	88	PRO	2.4
4	B	361	TRP	2.4
3	A	122	ARG	2.4
4	B	313	ASP	2.3
3	A	129	VAL	2.3
1	C	22	DG	2.3
3	A	28	VAL	2.2
3	A	98	LYS	2.2
3	A	91	ALA	2.2
2	D	1	DA	2.2
3	A	83	ILE	2.2
4	B	316	LYS	2.1
4	B	314	LEU	2.1
2	D	4	DG	2.0
3	A	128	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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.