



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:56 AM UTC

PDB ID : 1MDM / pdb_00001mdm
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

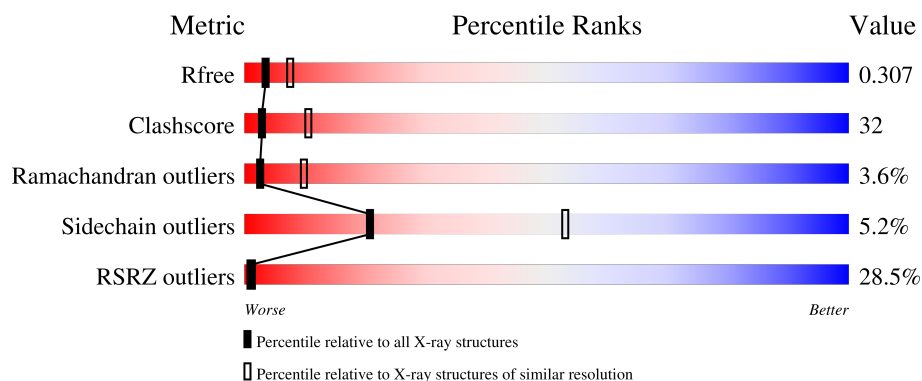
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
2	D	26	
3	A	149	
4	B	161	

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
1	C	26	Total	C	N	O	P	0	0	0
			533	253	98	157	25			

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

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

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

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

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

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

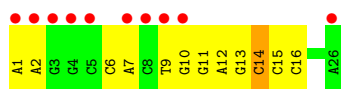
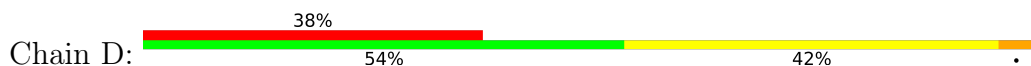
3 Residue-property plots [i](#)

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

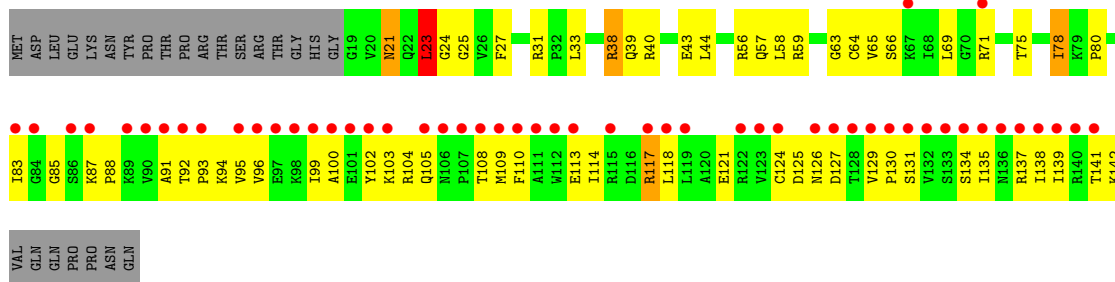
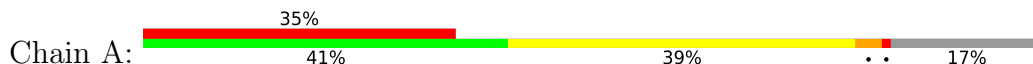
- Molecule 1: PAX5/ETS BINDING SITE ON THE MB-1 PROMOTER



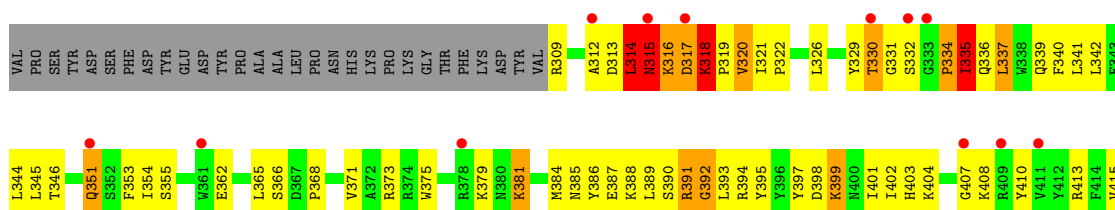
- Molecule 2: PAX5/ETS BINDING SITE ON THE MB-1 PROMOTER

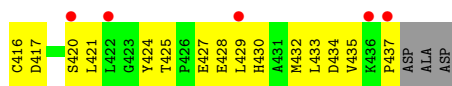


- Molecule 3: PAIRED BOX PROTEIN PAX-5



- 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, α , β , γ	77.27Å 171.23Å 44.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.03 – 2.80 32.03 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.3 (32.03-2.80) 87.3 (32.03-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.81Å)	Xtriage
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 ²)	55.7	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3054	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.37	0/597	0.74	0/921
2	D	0.35	0/591	0.69	0/909
3	A	0.49	0/980	1.06	4/1324 (0.3%)
4	B	0.82	1/1057 (0.1%)	1.22	17/1431 (1.2%)
All	All	0.58	1/3225 (0.0%)	1.00	21/4585 (0.5%)

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	-18.03	1.22	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	316	LYS	N-CA-C	10.51	133.19	110.80
4	B	317	ASP	N-CA-C	8.53	128.97	110.80
4	B	315	ASN	CA-C-N	7.69	136.23	121.54
4	B	315	ASN	C-N-CA	7.69	136.23	121.54
4	B	399	LYS	N-CA-C	-7.27	103.55	113.30
4	B	318	LYS	N-CA-C	7.16	125.63	109.81
3	A	38	ARG	N-CA-C	-6.99	103.66	111.28
3	A	78	ILE	N-CA-C	-6.82	106.35	112.90
4	B	316	LYS	CA-C-N	6.52	134.00	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	316	LYS	C-N-CA	6.52	134.00	121.54
4	B	416	CYS	N-CA-C	-6.24	102.49	110.53
4	B	392	GLY	N-CA-C	-6.16	105.36	112.50
4	B	437	PRO	N-CA-CB	5.91	109.50	103.00
4	B	320	VAL	N-CA-C	5.77	116.50	110.62
3	A	23	LEU	N-CA-C	-5.59	106.30	113.23
4	B	334	PRO	N-CD-CG	5.52	111.49	103.20
4	B	315	ASN	N-CA-C	5.38	122.27	110.80
3	A	126	ASN	N-CA-C	-5.29	106.86	113.15
4	B	381	LYS	CA-C-N	5.08	125.36	119.47
4	B	381	LYS	C-N-CA	5.08	125.36	119.47
4	B	351	GLN	N-CA-C	5.05	121.55	110.80

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

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	71	0
4	B	1030	0	1000	81	0
All	All	3054	0	2592	178	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 32.

All (178) 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
3:A:21:ASN:C	3:A:21:ASN:HD22	1.86	0.83
4:B:313:ASP:O	4:B:315:ASN:N	2.13	0.81
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
2:D:1:DA:H2''	2:D:2:DA:C8	2.26	0.71
4:B:326:LEU:CD1	4:B:330:THR:CG2	2.61	0.71
3:A:21:ASN:HD21	3:A:25:GLY:N	1.88	0.69
4:B:407:GLY:O	4:B:408:LYS:HG3	1.92	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:427:GLU:H	4:B:427:GLU:CD	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	4:B:432:MET:HE3	1.83	0.61
2:D:12:DA:H2''	2:D:13:DG:C8	2.37	0.60
3:A:63:GLY:O	3:A:66:SER:HB3	2.02	0.60
3:A:141:THR:O	3:A:142:LYS:HG3	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:H5'	1:C:17:DC:C6	2.34	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
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:424:TYR:CE2	4:B:432:MET:HE1	2.42	0.55
3:A:125:ASP:C	3:A:127:ASP:H	2.15	0.54
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:21:ASN:C	3:A:21:ASN:ND2	2.58	0.52
4:B:313:ASP:O	4:B:314:LEU:C	2.52	0.52
2:D:1:DA:H2'	2:D:1:DA:N3	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: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:57:GLN:C	3:A:59:ARG:H	2.20	0.49
3:A:71:ARG:O	3:A:75:THR:HB	2.13	0.49
3:A:94:LYS:HG3	3:A:95:VAL:H	1.78	0.49
3:A:103:LYS:HG3	3:A:139:ILE:HD12	1.94	0.49
4:B:346:THR:HA	4:B:433:LEU:HD11	1.93	0.49
2:D:14:DC:H2''	2:D:15:DC:C5	2.48	0.49
3:A:92:THR:CG2	3:A:93:PRO:HD2	2.41	0.49
3:A:92:THR:HG21	3:A:94:LYS:HZ3	1.78	0.49
4:B:337:LEU:HD22	4:B:337:LEU:C	2.38	0.49
4:B:362:GLU:HB2	4:B:413:ARG:CZ	2.43	0.48
4:B:391:ARG:HG3	4:B:391:ARG:O	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:CZ	4:B:373:ARG:HB2	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
3:A:105:GLN:CD	3:A:117:ARG:HH22	2.21	0.47
4:B:365:LEU:HB2	4:B:410:TYR:HB3	1.96	0.47
4:B:429:LEU:HA	4:B:432:MET:HE2	1.95	0.47
2:D:12:DA:H2''	2:D:13:DG:H8	1.80	0.46
1:C:10:DA:H2''	1:C:11:DT:H5'	1.97	0.46
3:A:31:ARG:HH21	3:A:83:ILE:HD12	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:DC:C2'	1:C:16:DT:H72	2.45	0.46
3:A:87:LYS:HE2	3:A:87:LYS:HA	1.97	0.46
1:C:10:DA:H1'	1:C:11:DT:H5''	1.99	0.45
3:A:94:LYS:CG	3:A:95:VAL:N	2.78	0.45
4:B:312:ALA:C	4:B:314:LEU:H	2.24	0.45
4:B:335:ILE:O	4:B:335:ILE:CG2	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
1:C:16:DT:H1'	1:C:17:DC:H5''	1.98	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
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
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:330:THR:CB	4:B:421:LEU:HD11	2.41	0.44
4:B:336:GLN:O	4:B:337:LEU:C	2.60	0.44
3:A:110:PHE:O	3:A:114:ILE:HG12	2.18	0.43
3:A:27:PHE:CD1	3:A:27:PHE:C	2.96	0.43
4:B:331:GLY:O	4:B:332:SER:OG	2.26	0.43
4:B:340:PHE:CE2	4:B:344:LEU:HD11	2.53	0.43
1:C:21:DT:H2''	1:C:22:DG:C8	2.54	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
4:B:386:TYR:O	4:B:387:GLU:C	2.60	0.43
2:D:16:DC:H5''	3:A:27:PHE:CD2	2.54	0.43
1:C:4:DC:H5''	4:B:404:LYS:HZ3	1.82	0.43
3:A:40:ARG:HD2	3:A:40:ARG:HA	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:71:ARG:HG2	3:A:71:ARG:HH11	1.84	0.42
1:C:25:DC:H2''	1:C:26:DT:C6	2.55	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
4:B:429:LEU:HA	4:B:432:MET:HE3	2.01	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:CD2	3:A:102:TYR:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:6:DC:H1'	2:D:7:DA:N7	2.36	0.41
2:D:10:DG:N2	3:A:85:GLY:O	2.54	0.41
3:A:21:ASN:ND2	3:A:24:GLY:N	2.69	0.41
3:A:129:VAL:HA	3:A:130:PRO:HD3	1.87	0.41
3:A:64:CYS:O	3:A:65:VAL:C	2.60	0.41
1:C:1:DT:H2''	1:C:2:DT:H72	2.04	0.40
1:C:15:DC:H2'	1:C:16:DT:H72	2.03	0.40
4:B:385:ASN:ND2	4:B:388:LYS:HE2	2.36	0.40
3:A:44:LEU:HD11	3:A:58:LEU:HD11	2.02	0.40
1:C:12:DG:O5'	1:C:12:DG:H2'	2.21	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	A	122/149 (82%)	110 (90%)	11 (9%)	1 (1%)	16	44
4	B	127/161 (79%)	98 (77%)	21 (16%)	8 (6%)	1	3
All	All	249/310 (80%)	208 (84%)	32 (13%)	9 (4%)	2	10

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

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Mol	Chain	Res	Type
4	B	314	LEU
4	B	330	THR
4	B	335	ILE
3	A	91	ALA

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	A	107/131 (82%)	103 (96%)	4 (4%)	30	65
4	B	104/140 (74%)	97 (93%)	7 (7%)	15	42
All	All	211/271 (78%)	200 (95%)	11 (5%)	21	53

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	21	ASN
3	A	23	LEU
3	A	108	THR
3	A	117	ARG
4	B	309	ARG
4	B	314	LEU
4	B	335	ILE
4	B	337	LEU
4	B	342	LEU
4	B	391	ARG
4	B	434	ASP

Sometimes 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	106	ASN
3	A	136	ASN

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Mol	Chain	Res	Type
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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	26/26 (100%)	1.05	8 (30%) 1 1	29, 54, 105, 124	0
2	D	26/26 (100%)	1.21	10 (38%) 1 0	26, 58, 124, 128	0
3	A	124/149 (83%)	1.61	52 (41%) 0 0	19, 74, 194, 200	0
4	B	129/161 (80%)	0.75	17 (13%) 7 6	17, 51, 112, 137	0
All	All	305/362 (84%)	1.16	87 (28%) 1 1	17, 57, 182, 200	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	99	ILE	9.9
3	A	132	VAL	7.2
3	A	133	SER	6.3
3	A	111	ALA	5.9
3	A	141	THR	5.7
4	B	437	PRO	5.2
4	B	330	THR	5.0
3	A	108	THR	4.9
2	D	1	DA	4.8
3	A	137	ARG	4.7
3	A	95	VAL	4.7
3	A	89	LYS	4.4
3	A	136	ASN	4.3
3	A	115	ARG	4.3
1	C	25	DC	4.1
3	A	109	MET	4.0
3	A	124	CYS	3.9
3	A	96	VAL	3.7
3	A	134	SER	3.7
3	A	102	TYR	3.7
3	A	112	TRP	3.5

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Mol	Chain	Res	Type	RSRZ
3	A	126	ASN	3.5
2	D	3	DG	3.5
3	A	138	ILE	3.5
3	A	118	LEU	3.5
2	D	8	DC	3.3
3	A	110	PHE	3.3
3	A	119	LEU	3.3
3	A	123	VAL	3.3
3	A	83	ILE	3.2
4	B	312	ALA	3.2
3	A	107	PRO	3.2
1	C	23	DG	3.1
2	D	26	DA	3.1
2	D	2	DA	3.1
1	C	22	DG	3.0
3	A	103	LYS	2.9
4	B	317	ASP	2.9
4	B	429	LEU	2.9
2	D	4	DG	2.9
4	B	315	ASN	2.9
3	A	131	SER	2.9
3	A	91	ALA	2.8
3	A	130	PRO	2.8
1	C	2	DT	2.8
1	C	26	DT	2.8
4	B	420	SER	2.7
3	A	92	THR	2.7
3	A	67	LYS	2.6
3	A	106	ASN	2.6
4	B	407	GLY	2.6
3	A	71	ARG	2.6
4	B	333	GLY	2.6
1	C	1	DT	2.5
3	A	90	VAL	2.5
4	B	378	ARG	2.5
4	B	409	ARG	2.5
1	C	24	DC	2.5
3	A	93	PRO	2.5
3	A	86	SER	2.5
3	A	139	ILE	2.5
3	A	97	GLU	2.5
4	B	411	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
4	B	351	GLN	2.4
3	A	87	LYS	2.4
1	C	20	DG	2.4
4	B	422	LEU	2.4
3	A	98	LYS	2.4
4	B	361	TRP	2.4
3	A	101	GLU	2.3
3	A	100	ALA	2.3
3	A	129	VAL	2.3
2	D	7	DA	2.3
2	D	5	DC	2.3
4	B	436	LYS	2.3
3	A	140	ARG	2.3
2	D	9	DT	2.2
3	A	135	ILE	2.2
3	A	128	THR	2.2
3	A	84	GLY	2.2
4	B	332	SER	2.2
3	A	105	GLN	2.1
3	A	122	ARG	2.1
3	A	117	ARG	2.1
3	A	127	ASP	2.1
3	A	113	GLU	2.1
2	D	10	DG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.