



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:59 PM UTC

PDB ID : 4XRS / pdb_00004xrs
Title : Heterodimeric complex of transcription factors MEIS1 and DLX3 on specific DNA
Authors : Jorma, A.; Yin, Y.; Nitta, K.R.; Dave, K.; Enge, M.; Kivioja, T.; Popov, A.; Morgunova, E.; Taipale, J.
Deposited on : 2015-01-21
Resolution : 3.50 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:

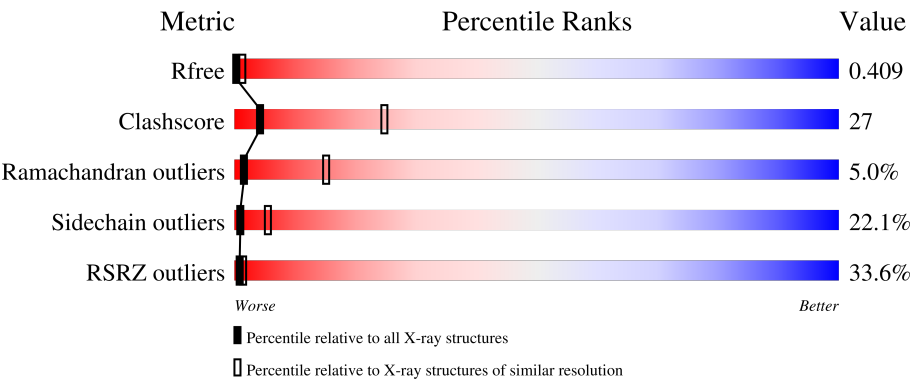
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	M	15	13% 47% 53%
2	D	17	47% 47% 53%
3	E	18	39% 44% 56%
4	L	17	41% 35% 59% 6%
5	A	58	34% 41% 43% 10% ...

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Mol	Chain	Length	Quality of chain
5	B	58	40%40%48%10%•
6	G	56	29%27%46%23%•
6	I	56	27%34%48%16%•

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3247 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 DNA (5'-D(P*CP*AP*AP*TP*TP*AP*TP*CP*CP*TP*GP*TP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	15	Total	C	N	O	P	0	0	0
			303	146	52	90	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	17	Total	C	N	O	P	0	0	0
			343	165	60	101	17			

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*TP*TP*GP*AP*CP*AP*GP*GP*AP*TP*AP*AP*TP*TP*GP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	18	Total	C	N	O	P	0	0	0
			374	179	67	110	18			

- Molecule 4 is a DNA chain called DNA (5'-D(P*TP*TP*GP*AP*CP*AP*GP*GP*AP*TP*AP*AP*TP*TP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	16	Total	C	N	O	P	0	0	0
			332	159	60	97	16			

- Molecule 5 is a protein called Homeobox protein Meis1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	56	Total	C	N	O	S	0	0	0
			468	301	87	78	2			
5	B	58	Total	C	N	O	S	0	0	0
			487	314	89	82	2			

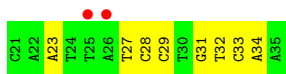
- Molecule 6 is a protein called Homeobox protein DLX-3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	56	Total	C	N	O	0	0	0
			472	304	90	78			
6	I	56	Total	C	N	O	0	0	0
			468	301	89	78			

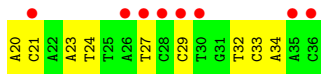
3 Residue-property plots [i](#)

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.

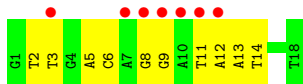
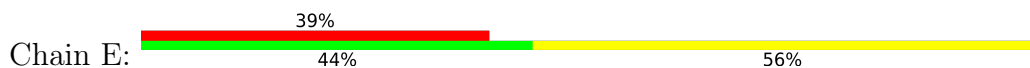
- Molecule 1: DNA (5'-D(P*CP*AP*AP*TP*TP*AP*TP*CP*CP*TP*GP*TP*CP*AP*A)-3')



- Molecule 2: DNA (5'-D(P*AP*CP*AP*AP*TP*TP*AP*TP*CP*CP*TP*GP*TP*CP*AP*AP*P*C)-3')



- Molecule 3: DNA (5'-D(P*GP*TP*TP*GP*AP*CP*AP*GP*GP*AP*TP*AP*AP*TP*TP*GP*TP*T)-3')

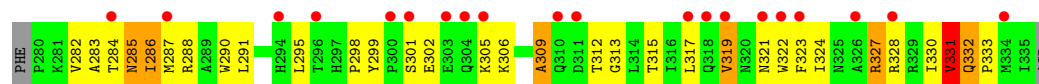


- Molecule 4: DNA (5'-D(P*TP*TP*GP*AP*CP*AP*GP*GP*AP*TP*AP*AP*TP*TP*GP*T)-3')



- Molecule 5: Homeobox protein Meis1





• Molecule 5: Homeobox protein Meis1



• Molecule 6: Homeobox protein DLX-3



• Molecule 6: Homeobox protein DLX-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.64Å 69.84Å 116.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.31 – 3.50 49.31 – 3.50	Depositor EDS
% Data completeness (in resolution range)	88.1 (49.31-3.50) 88.6 (49.31-3.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.96Å)	Xtriage
Refinement program	PHENIX phenix.refine: 1.9_1692	Depositor
R, R_{free}	0.331 , 0.359 0.390 , 0.409	Depositor DCC
R_{free} test set	529 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å ²)	101.7	Xtriage
Anisotropy	0.765	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 155.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.001 for k,h,-l	Xtriage
Reported twinning fraction	0.080 for k,h,-l	Depositor
Outliers	2 of 10985 reflections (0.018%)	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	3247	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1274e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [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	M	0.29	0/338	0.59	0/518
2	D	0.30	0/383	0.60	0/587
3	E	0.30	0/419	0.60	0/646
4	L	0.26	0/372	0.59	0/573
5	A	0.43	0/480	0.88	1/651 (0.2%)
5	B	0.47	0/500	1.05	2/679 (0.3%)
6	G	0.50	0/481	1.15	4/644 (0.6%)
6	I	0.47	0/477	0.93	2/640 (0.3%)
All	All	0.40	0/3450	0.84	9/4938 (0.2%)

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
5	B	0	1
6	G	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	279	PHE	CA-C-N	-7.49	112.06	119.78
5	B	279	PHE	C-N-CA	-7.49	112.06	119.78
6	G	175	ILE	N-CA-C	6.78	117.53	110.62
5	A	283	ALA	N-CA-C	-5.37	106.60	112.72
6	I	139	TYR	CA-C-N	5.09	130.86	121.70
6	I	139	TYR	C-N-CA	5.09	130.86	121.70
6	G	174	LYS	N-CA-C	-5.08	105.87	111.71
6	G	139	TYR	CA-C-N	5.04	130.77	121.70
6	G	139	TYR	C-N-CA	5.04	130.77	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	328	ARG	Peptide
6	G	181	ARG	Peptide

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	M	303	0	171	13	0
2	D	343	0	193	15	0
3	E	374	0	206	19	0
4	L	332	0	183	15	0
5	A	468	0	479	22	0
5	B	487	0	491	33	0
6	G	472	0	497	35	0
6	I	468	0	486	41	0
All	All	3247	0	2706	159	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 27.

All (159) 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)
6:I:156:LEU:O	6:I:160:ALA:N	2.03	0.91
5:A:309:ALA:O	5:A:313:GLY:N	2.01	0.91
4:L:13:DA:O3'	6:G:131:LYS:N	2.05	0.89
5:B:279:PHE:N	5:B:284:THR:HG1	1.72	0.87
3:E:12:DA:N7	6:I:179:ASN:ND2	2.29	0.81
5:B:309:ALA:O	5:B:313:GLY:N	2.15	0.79
5:B:305:LYS:O	5:B:309:ALA:N	2.15	0.79
3:E:11:DT:O2	6:I:133:ARG:NH2	2.17	0.77
6:I:159:ARG:NH2	6:I:170:GLN:O	2.17	0.77
4:L:12:DA:N3	6:G:133:ARG:NH2	2.32	0.76
5:A:302:GLU:OE2	5:A:305:LYS:NZ	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:141:LEU:O	6:I:144:LEU:HD23	1.88	0.73
6:I:144:LEU:HD22	6:I:176:TRP:CZ3	2.24	0.73
6:I:147:ARG:NH1	6:I:158:GLU:O	2.22	0.72
5:B:294:HIS:O	5:B:297:HIS:N	2.23	0.71
5:B:282:VAL:O	5:B:286:ILE:N	2.20	0.70
5:A:317:LEU:O	5:A:321:ASN:ND2	2.23	0.70
2:D:29:DC:H42	3:E:8:DG:N2	1.90	0.69
5:B:279:PHE:N	5:B:284:THR:OG1	2.25	0.69
6:I:154:LEU:HD12	6:I:177:PHE:HZ	1.58	0.69
2:D:24:DT:H71	3:E:13:DA:N1	2.09	0.67
6:G:154:LEU:HD21	6:G:158:GLU:CB	2.25	0.66
6:I:175:ILE:O	6:I:179:ASN:ND2	2.29	0.66
2:D:20:DA:OP2	6:I:174:LYS:NZ	2.30	0.65
3:E:13:DA:O3'	6:I:131:LYS:N	2.30	0.65
2:D:29:DC:O2	3:E:9:DG:N2	2.30	0.65
5:B:295:LEU:HD23	5:B:331:VAL:HG11	1.79	0.65
2:D:34:DA:N6	3:E:2:DT:O4	2.31	0.64
5:B:302:GLU:N	5:B:302:GLU:OE2	2.31	0.63
6:I:144:LEU:HD22	6:I:176:TRP:CH2	2.34	0.62
1:M:33:DC:N4	4:L:3:DT:O4	2.33	0.62
6:G:163:ALA:O	6:G:167:GLY:N	2.32	0.61
2:D:32:DT:O4	3:E:5:DA:N6	2.33	0.61
6:G:136:TYR:HB2	6:G:137:SER:HA	1.83	0.61
6:G:160:ALA:O	6:G:164:ALA:N	2.32	0.60
6:I:158:GLU:N	6:I:158:GLU:OE1	2.35	0.59
6:G:154:LEU:HD21	6:G:158:GLU:HB3	1.84	0.59
6:I:139:TYR:HA	6:I:141:LEU:H	1.68	0.59
5:B:295:LEU:HD22	5:B:295:LEU:C	2.28	0.58
1:M:32:DT:H72	1:M:33:DC:C2	2.39	0.57
5:B:303:GLU:O	5:B:307:GLN:N	2.30	0.56
6:I:156:LEU:O	6:I:159:ARG:N	2.39	0.56
6:G:166:LEU:N	6:G:166:LEU:HD12	2.22	0.55
2:D:20:DA:N7	2:D:21:DC:N4	2.55	0.55
6:G:154:LEU:HD21	6:G:158:GLU:HB2	1.87	0.55
5:A:305:LYS:O	5:A:309:ALA:N	2.38	0.55
6:I:162:LEU:HD21	6:I:166:LEU:HD11	1.87	0.55
4:L:11:DT:O2	6:G:133:ARG:NH1	2.37	0.54
5:B:279:PHE:CG	5:B:280:PRO:HD3	2.43	0.54
3:E:12:DA:O4'	6:I:133:ARG:NE	2.39	0.54
6:I:154:LEU:HD12	6:I:177:PHE:CZ	2.41	0.54
2:D:21:DC:OP2	6:I:181:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:33:DC:N4	4:L:4:DG:O6	2.36	0.53
2:D:27:DT:O2	6:I:133:ARG:NH1	2.41	0.53
5:B:297:HIS:ND1	5:B:297:HIS:O	2.41	0.53
5:B:305:LYS:NZ	5:B:320:ASN:OD1	2.28	0.52
5:A:291:LEU:HD13	5:A:323:PHE:HE1	1.75	0.52
6:I:134:THR:O	6:I:135:ILE:HD13	2.10	0.52
5:B:299:TYR:OH	6:I:135:ILE:O	2.20	0.51
6:I:136:TYR:N	6:I:136:TYR:CD1	2.76	0.51
5:A:324:ILE:HG22	5:A:327:ARG:HH21	1.76	0.51
6:G:139:TYR:CA	6:G:140:GLN:HB2	2.41	0.50
6:I:156:LEU:HD13	6:I:159:ARG:HB3	1.93	0.50
6:G:159:ARG:HA	6:G:162:LEU:HB3	1.94	0.50
2:D:23:DA:N6	3:E:14:DT:O4	2.44	0.50
4:L:16:DG:N2	4:L:17:DT:H72	2.26	0.50
6:G:147:ARG:O	6:G:151:ALA:N	2.40	0.50
1:M:34:DA:N3	4:L:4:DG:N2	2.60	0.49
6:G:165:GLN:C	6:G:166:LEU:HD12	2.37	0.49
5:A:299:TYR:OH	6:G:134:THR:N	2.45	0.49
5:A:284:THR:O	5:A:287:MET:N	2.46	0.49
6:G:139:TYR:HA	6:G:140:GLN:HB2	1.94	0.49
1:M:27:DT:O2	6:G:133:ARG:NH1	2.45	0.48
3:E:2:DT:H2'	3:E:3:DT:H5'	1.95	0.48
5:B:306:LYS:HA	5:B:309:ALA:HB3	1.95	0.48
5:A:285:ASN:N	5:A:285:ASN:OD1	2.45	0.48
6:G:142:ALA:HA	6:G:145:GLN:HG3	1.96	0.48
6:I:139:TYR:HA	6:I:140:GLN:HB2	1.96	0.48
5:A:284:THR:HG23	5:A:322:TRP:CH2	2.49	0.48
6:I:139:TYR:CD1	6:I:139:TYR:N	2.80	0.48
5:B:285:ASN:OD1	5:B:285:ASN:N	2.47	0.47
6:I:162:LEU:CD2	6:I:166:LEU:HD11	2.44	0.47
5:B:326:ALA:O	5:B:328:ARG:N	2.46	0.47
6:I:184:PHE:HA	6:I:186:LYS:N	2.29	0.47
6:G:144:LEU:O	6:G:147:ARG:N	2.47	0.47
6:G:132:PRO:O	6:G:134:THR:HG23	2.15	0.47
6:I:136:TYR:N	6:I:137:SER:HA	2.29	0.47
5:B:299:TYR:CE1	6:I:134:THR:HG23	2.50	0.46
6:G:146:ARG:O	6:G:150:LYS:N	2.44	0.46
5:A:298:PRO:HB2	5:A:327:ARG:NH2	2.30	0.46
6:G:138:SER:O	6:G:141:LEU:HD13	2.16	0.46
1:M:23:DA:H61	4:L:13:DA:N6	2.13	0.46
5:B:324:ILE:HA	5:B:327:ARG:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:136:TYR:N	6:G:137:SER:CB	2.79	0.46
6:G:178:GLN:HA	6:G:181:ARG:HD3	1.97	0.45
6:I:184:PHE:HA	6:I:185:LYS:HB2	1.98	0.45
4:L:15:DT:C2'	4:L:16:DG:H5''	2.46	0.45
5:B:295:LEU:HA	5:B:298:PRO:HG3	1.99	0.45
6:G:134:THR:O	6:G:134:THR:OG1	2.33	0.45
6:G:169:THR:HG22	6:G:172:GLN:HE21	1.81	0.45
6:I:154:LEU:HD22	6:I:155:ALA:H	1.80	0.45
3:E:6:DC:OP2	5:B:318:GLN:NE2	2.49	0.45
4:L:15:DT:H2'	4:L:16:DG:C8	2.51	0.45
5:A:309:ALA:O	5:A:312:THR:N	2.46	0.45
5:B:295:LEU:HD13	5:B:296:THR:H	1.81	0.45
4:L:15:DT:H2''	4:L:16:DG:H5''	1.98	0.45
5:A:287:MET:HB3	5:A:323:PHE:HE2	1.82	0.44
5:A:330:ILE:C	5:A:331:VAL:HG13	2.42	0.44
5:B:332:GLN:N	5:B:333:PRO:CD	2.80	0.44
1:M:31:DG:N2	1:M:32:DT:C4	2.85	0.44
1:M:23:DA:H61	4:L:13:DA:H62	1.66	0.44
5:B:279:PHE:HB3	5:B:280:PRO:CD	2.48	0.44
6:G:135:ILE:HG13	6:G:137:SER:HB2	1.99	0.44
6:I:184:PHE:CD1	6:I:184:PHE:N	2.85	0.44
1:M:29:DC:O2	4:L:9:DG:N2	2.50	0.43
5:B:290:TRP:CZ2	5:B:308:LEU:CD1	3.01	0.43
5:B:282:VAL:O	5:B:285:ASN:N	2.51	0.43
5:A:330:ILE:C	5:A:333:PRO:HD2	2.43	0.43
6:I:162:LEU:HA	6:I:165:GLN:HB3	2.01	0.43
6:G:135:ILE:HD12	6:G:135:ILE:HA	1.90	0.42
1:M:28:DC:N3	4:L:10:DA:C2	2.87	0.42
5:A:330:ILE:O	5:A:332:GLN:N	2.43	0.42
5:A:287:MET:HA	5:A:290:TRP:CD1	2.54	0.42
6:G:139:TYR:HA	6:G:141:LEU:H	1.84	0.42
6:G:168:LEU:HD23	6:G:168:LEU:N	2.34	0.42
6:I:136:TYR:CZ	6:I:168:LEU:HD11	2.54	0.42
6:I:145:GLN:HA	6:I:148:PHE:HD2	1.85	0.42
3:E:6:DC:P	5:B:318:GLN:HE22	2.42	0.42
6:G:138:SER:O	6:G:139:TYR:CG	2.72	0.42
3:E:12:DA:H2'	3:E:13:DA:O4'	2.19	0.42
6:I:165:GLN:HG2	6:I:166:LEU:HD23	2.02	0.42
5:A:306:LYS:HA	5:A:309:ALA:HB3	2.00	0.42
1:M:23:DA:N6	4:L:13:DA:N6	2.68	0.42
5:A:290:TRP:CE3	5:A:291:LEU:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:154:LEU:HB2	6:I:177:PHE:HE2	1.85	0.41
1:M:27:DT:O2	6:G:133:ARG:CZ	2.68	0.41
2:D:29:DC:H42	3:E:8:DG:H21	1.67	0.41
5:B:305:LYS:HB2	5:B:316:ILE:HD11	2.02	0.41
2:D:33:DC:H1'	2:D:34:DA:H5''	2.03	0.41
3:E:8:DG:C2	3:E:9:DG:C5	3.08	0.41
5:B:279:PHE:CB	5:B:280:PRO:CD	2.99	0.41
5:A:286:ILE:CG1	5:A:287:MET:N	2.83	0.41
2:D:33:DC:H2''	2:D:34:DA:C5'	2.50	0.41
5:B:292:PHE:O	5:B:295:LEU:HD12	2.20	0.41
1:M:32:DT:H72	1:M:33:DC:N3	2.36	0.41
6:G:139:TYR:N	6:G:140:GLN:HB2	2.36	0.41
2:D:34:DA:H61	3:E:2:DT:C7	2.34	0.41
3:E:11:DT:H4'	3:E:12:DA:OP1	2.20	0.41
6:G:154:LEU:HG	6:G:155:ALA:N	2.35	0.41
6:G:163:ALA:CA	6:G:166:LEU:HD13	2.51	0.41
6:I:184:PHE:HB3	6:I:186:LYS:CA	2.51	0.41
5:A:315:THR:O	5:A:319:VAL:HG23	2.21	0.41
5:A:321:ASN:HA	5:A:324:ILE:HG12	2.03	0.41
5:B:297:HIS:HA	5:B:299:TYR:CE2	2.55	0.41
3:E:12:DA:N7	6:I:179:ASN:CG	2.79	0.40
5:B:279:PHE:HB3	5:B:280:PRO:HD2	2.04	0.40
5:B:321:ASN:OD1	5:B:321:ASN:N	2.54	0.40
6:I:154:LEU:CD2	6:I:155:ALA:H	2.35	0.40
2:D:33:DC:H2''	2:D:34:DA:H5''	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
5	A	54/58 (93%)	45 (83%)	7 (13%)	2 (4%)	2 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B	56/58 (97%)	51 (91%)	4 (7%)	1 (2%)	6	34
6	G	54/56 (96%)	42 (78%)	8 (15%)	4 (7%)	1	9
6	I	54/56 (96%)	38 (70%)	12 (22%)	4 (7%)	1	9
All	All	218/228 (96%)	176 (81%)	31 (14%)	11 (5%)	1	15

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	138	SER
6	G	140	GLN
5	A	309	ALA
6	G	134	THR
6	G	160	ALA
6	I	150	LYS
6	I	167	GLY
6	I	177	PHE
5	B	328	ARG
5	A	331	VAL
6	I	132	PRO

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	
5	A	51/53 (96%)	40 (78%)	11 (22%)	1	6
5	B	53/53 (100%)	46 (87%)	7 (13%)	4	20
6	G	48/48 (100%)	32 (67%)	16 (33%)	0	2
6	I	47/48 (98%)	37 (79%)	10 (21%)	1	6
All	All	199/202 (98%)	155 (78%)	44 (22%)	1	5

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	282	VAL
5	A	285	ASN
5	A	286	ILE
5	A	288	ARG
5	A	295	LEU
5	A	301	SER
5	A	319	VAL
5	A	327	ARG
5	A	328	ARG
5	A	331	VAL
5	A	332	GLN
5	B	285	ASN
5	B	294	HIS
5	B	295	LEU
5	B	302	GLU
5	B	317	LEU
5	B	319	VAL
5	B	321	ASN
6	G	131	LYS
6	G	135	ILE
6	G	137	SER
6	G	138	SER
6	G	146	ARG
6	G	158	GLU
6	G	161	GLU
6	G	162	LEU
6	G	166	LEU
6	G	168	LEU
6	G	173	VAL
6	G	175	ILE
6	G	181	ARG
6	G	182	SER
6	G	183	LYS
6	G	186	LYS
6	I	133	ARG
6	I	134	THR
6	I	135	ILE
6	I	136	TYR
6	I	139	TYR
6	I	140	GLN
6	I	154	LEU
6	I	162	LEU
6	I	169	THR

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Mol	Chain	Res	Type
6	I	184	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	320	ASN
5	A	321	ASN
5	B	318	GLN
6	G	172	GLN
6	I	140	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	M	15/15 (100%)	1.46	2 (13%) 7 6	109, 137, 159, 169	0
2	D	17/17 (100%)	1.91	8 (47%) 0 1	101, 125, 146, 149	0
3	E	18/18 (100%)	1.87	7 (38%) 1 1	114, 124, 153, 158	0
4	L	16/17 (94%)	1.91	7 (43%) 0 1	118, 141, 163, 164	0
5	A	56/58 (96%)	1.80	20 (35%) 1 1	121, 141, 173, 190	0
5	B	58/58 (100%)	2.13	23 (39%) 1 1	111, 143, 165, 176	0
6	G	56/56 (100%)	1.70	16 (28%) 1 1	115, 134, 146, 161	0
6	I	56/56 (100%)	1.66	15 (26%) 1 2	113, 132, 150, 152	0
All	All	292/295 (98%)	1.82	98 (33%) 1 1	101, 136, 163, 190	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	326	ALA	10.7
6	G	161	GLU	5.9
5	A	326	ALA	5.5
6	G	173	VAL	5.1
5	A	304	GLN	4.9
5	B	322	TRP	4.8
5	B	328	ARG	4.8
6	I	163	ALA	4.7
5	A	321	ASN	4.5
6	I	173	VAL	4.4
5	A	300	PRO	4.4
5	A	319	VAL	4.3
5	B	323	PHE	4.0
6	G	165	GLN	4.0
6	G	171	THR	4.0
5	B	303	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
6	G	136	TYR	3.7
2	D	30	DT	3.6
6	G	179	ASN	3.6
6	I	134	THR	3.5
5	A	323	PHE	3.5
5	A	317	LEU	3.5
6	I	148	PHE	3.4
5	B	284	THR	3.4
5	B	319	VAL	3.4
5	B	289	ALA	3.3
5	B	287	MET	3.3
6	G	178	GLN	3.2
4	L	17	DT	3.2
5	B	321	ASN	3.2
4	L	6	DC	3.1
6	I	175	ILE	3.1
5	B	286	ILE	3.1
5	B	280	PRO	3.1
1	M	26	DA	3.0
6	I	186	LYS	3.0
6	G	172	GLN	3.0
5	B	305	LYS	2.9
2	D	36	DC	2.9
3	E	7	DA	2.9
5	B	283	ALA	2.8
3	E	11	DT	2.8
6	I	135	ILE	2.8
6	I	149	GLN	2.7
6	I	154	LEU	2.7
6	I	180	ARG	2.7
5	A	305	LYS	2.7
6	I	177	PHE	2.6
5	A	318	GLN	2.6
6	I	167	GLY	2.6
4	L	9	DG	2.6
4	L	11	DT	2.6
5	A	287	MET	2.6
2	D	29	DC	2.6
5	B	315	THR	2.6
6	G	137	SER	2.5
5	A	334	MET	2.5
6	G	142	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
4	L	14	DT	2.5
5	B	327	ARG	2.5
3	E	12	DA	2.4
5	A	296	THR	2.4
5	B	330	ILE	2.4
5	A	301	SER	2.4
5	A	303	GLU	2.4
5	A	294	HIS	2.3
5	B	313	GLY	2.3
3	E	8	DG	2.3
5	B	285	ASN	2.3
6	G	141	LEU	2.2
2	D	35	DA	2.2
5	A	328	ARG	2.2
5	A	322	TRP	2.2
6	I	176	TRP	2.2
6	G	164	ALA	2.2
3	E	10	DA	2.2
6	I	179	ASN	2.2
2	D	21	DC	2.2
6	I	160	ALA	2.2
6	G	140	GLN	2.2
5	B	279	PHE	2.2
2	D	27	DT	2.2
3	E	3	DT	2.2
2	D	28	DC	2.2
3	E	9	DG	2.2
5	B	304	GLN	2.1
5	A	310	GLN	2.1
5	B	336	ASP	2.1
5	A	284	THR	2.1
6	G	182	SER	2.1
5	B	320	ASN	2.1
1	M	25	DT	2.1
2	D	26	DA	2.1
4	L	12	DA	2.1
6	G	143	ALA	2.0
5	A	311	ASP	2.0
6	G	148	PHE	2.0
4	L	7	DA	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.