



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 12:45 PM EDT

PDB ID : 2IT0 / pdb\_00002it0  
Title : Crystal structure of a two-domain IdeR-DNA complex crystal form II  
Authors : Wisedchaisri, G.; Chou, C.J.; Wu, M.; Roach, C.; Rice, A.E.; Holmes, R.K.;  
Beeson, C.; Hol, W.G.  
Deposited on : 2006-10-18  
Resolution : 2.60 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.

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 Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

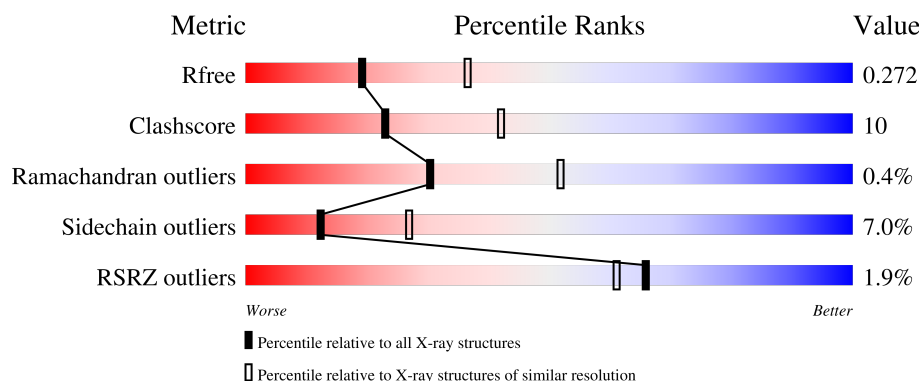
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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  $\geq 3$ , 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	E	33	<div> <div>9%</div> <div>45%</div> <div>52%</div> <div>.</div> </div>
2	F	33	<div> <div>12%</div> <div>55%</div> <div>45%</div> </div>
3	A	157	<div> <div>%</div> <div>73%</div> <div>17%</div> <div>8%</div> <div>.</div> </div>
3	B	157	<div> <div>%</div> <div>67%</div> <div>24%</div> <div>8%</div> <div>.</div> </div>
3	C	157	<div> <div>%</div> <div>63%</div> <div>20%</div> <div>13%</div> <div>.</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	157	<div><div><div>%</div><div><div></div></div><div>64%</div><div>22%</div><div>•</div><div>13%</div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5916 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 mbtA/mbtB operator strand 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	33	Total	C	N	O	P	0	0	0
			670	321	117	200	32			

- Molecule 2 is a DNA chain called mbtA/mbtB operator strand 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	33	Total	C	N	O	P	0	0	0
			677	322	131	192	32			

- Molecule 3 is a protein called Iron-dependent repressor ideR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	145	Total	C	N	O	S	0	0	0
			1151	720	209	217	5			
3	B	145	Total	C	N	O	S	0	0	0
			1155	722	209	219	5			
3	C	137	Total	C	N	O	S	0	0	0
			1089	678	200	206	5			
3	D	137	Total	C	N	O	S	0	0	0
			1089	678	200	206	5			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ALA	-	expression tag	UNP P0A672
A	142	SER	-	expression tag	UNP P0A672
A	143	GLU	-	expression tag	UNP P0A672
A	144	ASN	-	expression tag	UNP P0A672
A	145	LEU	-	expression tag	UNP P0A672
A	146	TYR	-	expression tag	UNP P0A672
A	147	PHE	-	expression tag	UNP P0A672
A	148	GLN	-	expression tag	UNP P0A672

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	149	GLY	-	expression tag	UNP P0A672
A	150	GLY	-	expression tag	UNP P0A672
A	151	GLY	-	expression tag	UNP P0A672
A	152	HIS	-	expression tag	UNP P0A672
A	153	HIS	-	expression tag	UNP P0A672
A	154	HIS	-	expression tag	UNP P0A672
A	155	HIS	-	expression tag	UNP P0A672
A	156	HIS	-	expression tag	UNP P0A672
A	157	HIS	-	expression tag	UNP P0A672
B	141	ALA	-	expression tag	UNP P0A672
B	142	SER	-	expression tag	UNP P0A672
B	143	GLU	-	expression tag	UNP P0A672
B	144	ASN	-	expression tag	UNP P0A672
B	145	LEU	-	expression tag	UNP P0A672
B	146	TYR	-	expression tag	UNP P0A672
B	147	PHE	-	expression tag	UNP P0A672
B	148	GLN	-	expression tag	UNP P0A672
B	149	GLY	-	expression tag	UNP P0A672
B	150	GLY	-	expression tag	UNP P0A672
B	151	GLY	-	expression tag	UNP P0A672
B	152	HIS	-	expression tag	UNP P0A672
B	153	HIS	-	expression tag	UNP P0A672
B	154	HIS	-	expression tag	UNP P0A672
B	155	HIS	-	expression tag	UNP P0A672
B	156	HIS	-	expression tag	UNP P0A672
B	157	HIS	-	expression tag	UNP P0A672
C	141	ALA	-	expression tag	UNP P0A672
C	142	SER	-	expression tag	UNP P0A672
C	143	GLU	-	expression tag	UNP P0A672
C	144	ASN	-	expression tag	UNP P0A672
C	145	LEU	-	expression tag	UNP P0A672
C	146	TYR	-	expression tag	UNP P0A672
C	147	PHE	-	expression tag	UNP P0A672
C	148	GLN	-	expression tag	UNP P0A672
C	149	GLY	-	expression tag	UNP P0A672
C	150	GLY	-	expression tag	UNP P0A672
C	151	GLY	-	expression tag	UNP P0A672
C	152	HIS	-	expression tag	UNP P0A672
C	153	HIS	-	expression tag	UNP P0A672
C	154	HIS	-	expression tag	UNP P0A672
C	155	HIS	-	expression tag	UNP P0A672
C	156	HIS	-	expression tag	UNP P0A672

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	157	HIS	-	expression tag	UNP P0A672
D	141	ALA	-	expression tag	UNP P0A672
D	142	SER	-	expression tag	UNP P0A672
D	143	GLU	-	expression tag	UNP P0A672
D	144	ASN	-	expression tag	UNP P0A672
D	145	LEU	-	expression tag	UNP P0A672
D	146	TYR	-	expression tag	UNP P0A672
D	147	PHE	-	expression tag	UNP P0A672
D	148	GLN	-	expression tag	UNP P0A672
D	149	GLY	-	expression tag	UNP P0A672
D	150	GLY	-	expression tag	UNP P0A672
D	151	GLY	-	expression tag	UNP P0A672
D	152	HIS	-	expression tag	UNP P0A672
D	153	HIS	-	expression tag	UNP P0A672
D	154	HIS	-	expression tag	UNP P0A672
D	155	HIS	-	expression tag	UNP P0A672
D	156	HIS	-	expression tag	UNP P0A672
D	157	HIS	-	expression tag	UNP P0A672

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Ni 3 3	0	0
4	B	3	Total Ni 3 3	0	0
4	C	3	Total Ni 3 3	0	0
4	D	3	Total Ni 3 3	0	0

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	4	Total O 4 4	0	0
6	F	4	Total O 4 4	0	0

*Continued on next page...*

*Continued from previous page...*

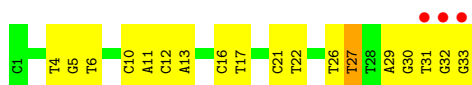
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total 6	O 6	0	0
6	B	10	Total 10	O 10	0	0
6	C	4	Total 4	O 4	0	0
6	D	5	Total 5	O 5	0	0



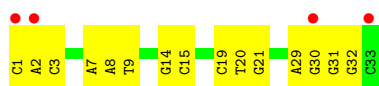
### 3 Residue-property plots [i](#)

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.

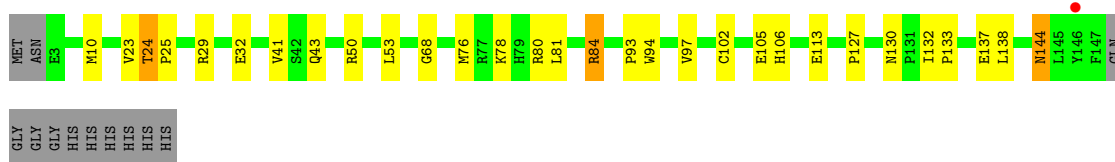
- Molecule 1: mbtA/mbtB operator strand 1



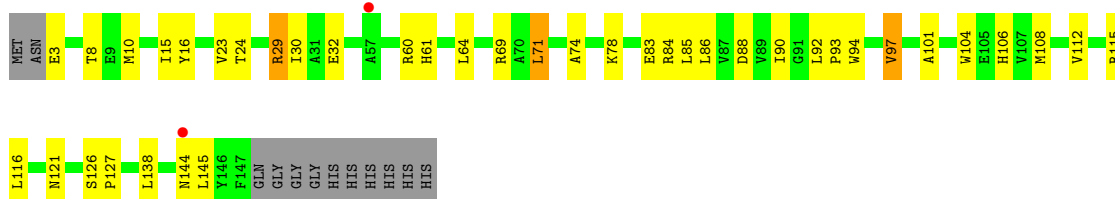
- Molecule 2: mbtA/mbtB operator strand 2



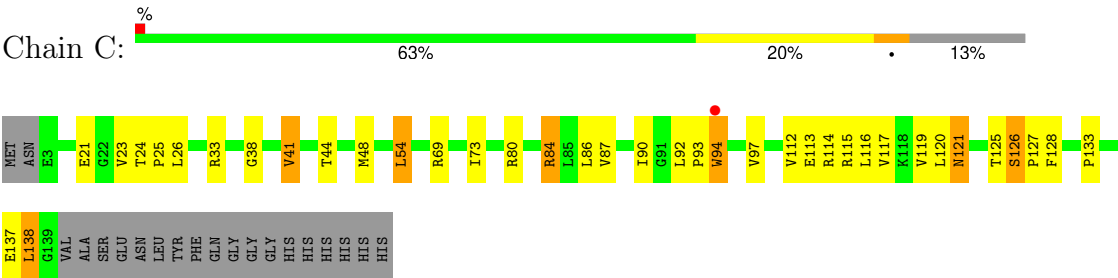
- Molecule 3: Iron-dependent repressor ideR



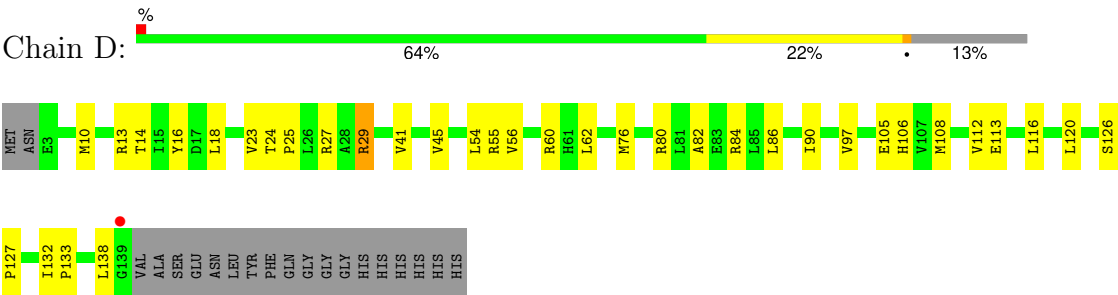
- Molecule 3: Iron-dependent repressor ideR



- Molecule 3: Iron-dependent repressor ideR



• Molecule 3: Iron-dependent repressor ideR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.01Å 70.36Å 79.57Å 108.95° 103.08° 94.84°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-2.60) 96.3 (50.00-2.60)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.03 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.226 , 0.273 0.227 , 0.272	Depositor DCC
$R_{free}$ test set	1596 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.7	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5916	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, ACT

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	E	0.32	0/749	1.04	2/1154 (0.2%)
2	F	0.31	0/761	0.93	0/1173
3	A	0.50	0/1170	0.81	0/1587
3	B	0.50	0/1174	0.82	0/1592
3	C	0.47	0/1106	0.81	0/1499
3	D	0.47	0/1106	0.78	0/1499
All	All	0.45	0/6066	0.86	2/8504 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	27	DT	C1'-O4'-C4'	-6.05	100.62	109.70
1	E	27	DT	N1-C1'-C2'	5.39	121.58	113.50

There are no chirality outliers.

There are no planarity outliers.

### 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	E	670	0	375	14	0
2	F	677	0	371	17	0
3	A	1151	0	1157	18	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1155	0	1161	27	0
3	C	1089	0	1101	24	0
3	D	1089	0	1101	21	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	A	12	0	9	0	0
5	B	8	0	6	1	0
5	C	12	0	9	0	0
5	D	8	0	6	0	0
6	A	6	0	0	1	0
6	B	10	0	0	3	0
6	C	4	0	0	0	0
6	D	5	0	0	0	0
6	E	4	0	0	0	0
6	F	4	0	0	0	0
All	All	5916	0	5296	113	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 10.

All (113) 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)
3:C:80:ARG:HG2	3:C:126:SER:HB2	1.45	0.96
3:D:16:TYR:HD1	3:D:76:MET:HE2	1.39	0.87
3:D:16:TYR:CD1	3:D:76:MET:HE2	2.10	0.84
3:C:92:LEU:HD12	3:C:93:PRO:HD2	1.67	0.75
3:C:114:ARG:HG3	3:C:138:LEU:HD22	1.69	0.75
2:F:14:DG:H2''	2:F:15:DC:H5'	1.68	0.74
3:A:78:LYS:NZ	3:A:113:GLU:OE2	2.20	0.72
1:E:29:DA:H2''	1:E:30:DG:OP2	1.89	0.71
3:C:94:TRP:O	3:C:97:VAL:HG22	1.89	0.71
1:E:5:DG:H2'	1:E:6:DT:H71	1.73	0.69
1:E:11:DA:H2''	1:E:12:DC:H5'	1.74	0.68
3:C:120:LEU:O	3:C:121:ASN:HB2	1.98	0.63
2:F:30:DG:H2''	2:F:31:DG:OP2	1.99	0.62
3:B:61:HIS:CE1	5:B:2002:ACT:O	2.51	0.62
3:A:137:GLU:OE1	3:A:137:GLU:N	2.29	0.62
1:E:33:DG:OP2	1:E:33:DG:H8	1.83	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:ILE:HG23	3:C:133:PRO:HB2	1.83	0.60
3:C:21:GLU:OE1	3:C:33:ARG:NH2	2.31	0.60
3:A:29:ARG:HH11	3:A:32:GLU:CD	2.10	0.60
2:F:7:DA:H4'	3:B:60:ARG:HH22	1.67	0.59
1:E:30:DG:H2''	1:E:31:DT:H72	1.84	0.59
3:B:74:ALA:O	3:B:78:LYS:HG3	2.03	0.58
3:B:3:GLU:HB3	6:B:2007:HOH:O	2.04	0.57
3:D:76:MET:HG2	3:D:133:PRO:HG3	1.87	0.56
2:F:2:DA:H2''	2:F:3:DC:OP2	2.06	0.55
3:D:86:LEU:HD23	3:D:90:ILE:HD12	1.89	0.55
3:C:87:VAL:HG22	3:C:97:VAL:HG11	1.88	0.55
2:F:2:DA:H1'	2:F:3:DC:O5'	2.07	0.55
3:A:43:GLN:NE2	6:A:2004:HOH:O	2.40	0.54
2:F:29:DA:H2'	2:F:29:DA:OP2	2.08	0.54
3:D:82:ALA:O	3:D:86:LEU:HG	2.08	0.54
3:D:84:ARG:HB3	3:D:120:LEU:HD13	1.90	0.54
3:B:94:TRP:CH2	3:B:127:PRO:HB2	2.43	0.53
3:C:113:GLU:O	3:C:117:VAL:HG23	2.07	0.53
1:E:32:DG:H2''	1:E:33:DG:OP2	2.09	0.53
3:B:104:TRP:O	3:B:108:MET:HG3	2.08	0.52
2:F:2:DA:H2'	2:F:2:DA:OP2	2.08	0.52
3:C:54:LEU:HD12	3:C:54:LEU:C	2.35	0.52
2:F:7:DA:OP1	3:B:29:ARG:NH2	2.44	0.51
3:A:93:PRO:HD3	3:B:115:ARG:CZ	2.40	0.51
2:F:31:DG:H2''	2:F:32:DG:OP2	2.11	0.50
3:D:27:ARG:HG3	3:D:62:LEU:HD11	1.94	0.50
3:D:80:ARG:HG2	3:D:126:SER:HB3	1.94	0.49
3:B:60:ARG:NE	6:B:2006:HOH:O	2.45	0.48
3:B:86:LEU:HA	3:B:90:ILE:HB	1.96	0.48
3:C:80:ARG:HG2	3:C:126:SER:CB	2.32	0.48
1:E:16:DC:H2'	1:E:17:DT:C6	2.49	0.48
2:F:7:DA:H1'	2:F:8:DA:H5'	1.95	0.48
2:F:19:DC:H2''	2:F:20:DT:H5'	1.95	0.47
3:B:8:THR:HB	6:B:2005:HOH:O	2.13	0.47
3:C:115:ARG:O	3:C:119:VAL:HG23	2.13	0.47
3:B:94:TRP:CZ3	3:B:127:PRO:HB2	2.48	0.47
3:C:112:VAL:O	3:C:116:LEU:HG	2.14	0.47
3:A:93:PRO:HD3	3:B:115:ARG:NE	2.30	0.47
3:A:76:MET:CG	3:A:133:PRO:HG3	2.45	0.47
3:A:76:MET:HG2	3:A:133:PRO:HG3	1.96	0.47
3:A:80:ARG:NH1	3:A:130:ASN:HB3	2.30	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:8:DA:H2''	2:F:9:DT:H71	1.96	0.47
3:D:108:MET:HE2	3:D:108:MET:HB3	1.79	0.47
3:C:114:ARG:HG3	3:C:138:LEU:CD2	2.44	0.46
3:C:69:ARG:O	3:C:73:ILE:HG13	2.15	0.46
2:F:1:DC:H2''	2:F:2:DA:OP2	2.14	0.46
2:F:8:DA:H5''	3:B:60:ARG:HD2	1.98	0.46
2:F:7:DA:H4'	3:B:60:ARG:NH2	2.29	0.46
3:C:87:VAL:CG2	3:C:97:VAL:HG11	2.44	0.46
3:D:14:THR:O	3:D:18:LEU:HG	2.16	0.45
3:D:108:MET:HE3	3:D:112:VAL:HG12	1.98	0.45
1:E:21:DC:H2'	1:E:22:DT:C6	2.51	0.45
3:D:80:ARG:HB3	3:D:132:ILE:HG12	1.97	0.45
3:A:105:GLU:HG3	3:A:106:HIS:CE1	2.51	0.45
3:B:92:LEU:HD12	3:B:93:PRO:HD2	1.98	0.45
3:D:108:MET:HE2	3:D:113:GLU:HG3	1.98	0.45
3:B:16:TYR:HE2	3:B:69:ARG:HH12	1.63	0.45
3:B:94:TRP:HA	3:B:97:VAL:HG13	1.98	0.45
3:B:83:GLU:HG3	3:B:101:ALA:CB	2.48	0.44
3:A:144:ASN:ND2	3:A:144:ASN:C	2.75	0.44
3:D:112:VAL:O	3:D:116:LEU:HG	2.18	0.44
1:E:10:DC:H2'	1:E:11:DA:C8	2.51	0.44
3:C:84:ARG:HA	3:C:127:PRO:HG3	1.99	0.44
2:F:14:DG:C2'	2:F:15:DC:H5'	2.43	0.44
3:B:15:ILE:HG21	3:B:64:LEU:HD21	1.99	0.44
3:B:29:ARG:NH1	3:B:32:GLU:OE1	2.51	0.44
3:B:84:ARG:NE	3:B:88:ASP:OD2	2.45	0.44
3:C:24:THR:HA	3:C:25:PRO:HD3	1.83	0.43
3:A:10:MET:HE1	3:A:102:CYS:SG	2.58	0.43
3:A:29:ARG:NE	3:A:29:ARG:HA	2.34	0.43
3:C:126:SER:C	3:C:128:PHE:H	2.26	0.43
3:D:24:THR:HA	3:D:25:PRO:HD3	1.77	0.43
1:E:26:DT:H2''	1:E:27:DT:H6	1.84	0.43
3:A:81:LEU:HD23	3:A:132:ILE:HD13	2.01	0.42
3:B:85:LEU:HD13	3:B:116:LEU:CD2	2.49	0.42
3:A:53:LEU:O	3:A:68:GLY:HA3	2.19	0.42
3:B:10:MET:SD	3:B:106:HIS:CE1	3.11	0.42
1:E:31:DT:H2''	1:E:32:DG:OP2	2.18	0.42
3:D:56:VAL:HG12	3:D:60:ARG:HA	2.01	0.42
3:A:24:THR:HA	3:A:25:PRO:HD3	1.76	0.42
3:C:120:LEU:O	3:C:121:ASN:CB	2.67	0.42
3:C:38:GLY:O	3:C:41:VAL:HG22	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:84:ARG:HG2	3:A:127:PRO:HD3	2.01	0.41
1:E:13:DA:C2	2:F:21:DG:C2	3.08	0.41
3:C:24:THR:HG22	3:C:26:LEU:HG	2.01	0.41
3:C:86:LEU:HD23	3:C:90:ILE:HD12	2.02	0.41
3:D:13:ARG:HD3	3:D:105:GLU:OE1	2.20	0.41
3:D:84:ARG:HG2	3:D:127:PRO:HD3	2.03	0.41
3:C:44:THR:O	3:C:48:MET:HG3	2.20	0.41
1:E:4:DT:OP1	3:D:29:ARG:NH2	2.53	0.41
1:E:5:DG:H2'	1:E:6:DT:C6	2.56	0.41
3:A:50:ARG:O	3:A:50:ARG:HG2	2.19	0.41
3:B:71:LEU:HD23	3:B:71:LEU:HA	1.95	0.40
3:B:29:ARG:NH1	3:B:32:GLU:CD	2.79	0.40
3:B:83:GLU:HG3	3:B:101:ALA:HB2	2.03	0.40
3:D:45:VAL:HG13	3:D:54:LEU:HD11	2.04	0.40
3:D:10:MET:SD	3:D:106:HIS:CE1	3.14	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	143/157 (91%)	139 (97%)	4 (3%)	0	100	100
3	B	143/157 (91%)	140 (98%)	3 (2%)	0	100	100
3	C	135/157 (86%)	125 (93%)	8 (6%)	2 (2%)	8	18
3	D	135/157 (86%)	123 (91%)	12 (9%)	0	100	100
All	All	556/628 (88%)	527 (95%)	27 (5%)	2 (0%)	30	52

All (2) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
3	C	94	TRP
3	C	121	ASN

### 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	125/135 (93%)	117 (94%)	8 (6%)	14	32
3	B	126/135 (93%)	114 (90%)	12 (10%)	7	14
3	C	119/135 (88%)	111 (93%)	8 (7%)	13	29
3	D	119/135 (88%)	113 (95%)	6 (5%)	20	43
All	All	489/540 (91%)	455 (93%)	34 (7%)	12	27

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	23	VAL
3	A	24	THR
3	A	41	VAL
3	A	84	ARG
3	A	94	TRP
3	A	97	VAL
3	A	138	LEU
3	A	144	ASN
3	B	23	VAL
3	B	24	THR
3	B	29	ARG
3	B	30	ILE
3	B	71	LEU
3	B	97	VAL
3	B	112	VAL
3	B	121	ASN
3	B	126	SER
3	B	138	LEU
3	B	144	ASN
3	B	145	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	23	VAL
3	C	41	VAL
3	C	54	LEU
3	C	84	ARG
3	C	125	THR
3	C	126	SER
3	C	137	GLU
3	C	138	LEU
3	D	23	VAL
3	D	29	ARG
3	D	41	VAL
3	D	55	ARG
3	D	97	VAL
3	D	138	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	43	GLN
3	A	130	ASN
3	A	144	ASN

### 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](#)

Of 22 ligands modelled in this entry, 12 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	ACT	A	2001	4	3,3,3	0.75	0	3,3,3	1.55	1 (33%)
5	ACT	B	2001	4	3,3,3	0.82	0	3,3,3	1.42	0
5	ACT	C	2003	4	3,3,3	0.74	0	3,3,3	1.59	0
5	ACT	A	2002	4	3,3,3	0.85	0	3,3,3	1.34	0
5	ACT	B	2002	4	3,3,3	0.85	0	3,3,3	1.66	1 (33%)
5	ACT	C	2002	4	3,3,3	0.89	0	3,3,3	1.33	0
5	ACT	A	2003	4	3,3,3	0.89	0	3,3,3	1.11	0
5	ACT	D	2002	4	3,3,3	0.93	0	3,3,3	1.35	0
5	ACT	C	2001	4	3,3,3	0.79	0	3,3,3	1.48	0
5	ACT	D	2001	4	3,3,3	0.83	0	3,3,3	1.50	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2002	ACT	OXT-C-O	-2.18	113.92	122.03
5	A	2001	ACT	OXT-C-CH3	2.04	123.60	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2002	ACT	1	0

## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	E	33/33 (100%)	0.00	3 (9%) 16 13	10, 27, 62, 65	0
2	F	33/33 (100%)	0.10	4 (12%) 10 8	12, 24, 66, 71	0
3	A	145/157 (92%)	-0.16	1 (0%) 84 81	10, 21, 32, 39	0
3	B	145/157 (92%)	-0.04	2 (1%) 73 68	10, 22, 37, 41	0
3	C	137/157 (87%)	-0.11	1 (0%) 84 81	12, 24, 34, 43	0
3	D	137/157 (87%)	0.02	1 (0%) 84 81	17, 24, 35, 39	0
All	All	630/694 (90%)	-0.06	12 (1%) 66 61	10, 23, 38, 71	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1	DC	3.0
1	E	33	DG	2.8
1	E	32	DG	2.7
3	C	94	TRP	2.4
3	D	139	GLY	2.4
2	F	33	DC	2.3
2	F	30	DG	2.2
3	A	146	TYR	2.1
3	B	144	ASN	2.1
2	F	2	DA	2.1
1	E	31	DT	2.1
3	B	57	ALA	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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ACT	A	2001	4/4	0.73	0.23	24,25,26,27	0
5	ACT	D	2002	4/4	0.73	0.19	26,27,28,29	0
5	ACT	C	2002	4/4	0.78	0.17	21,22,22,23	0
5	ACT	C	2001	4/4	0.79	0.27	38,39,39,40	0
5	ACT	D	2001	4/4	0.80	0.19	28,28,29,30	0
5	ACT	A	2002	4/4	0.80	0.28	40,40,41,41	0
5	ACT	B	2001	4/4	0.83	0.18	16,16,18,18	0
5	ACT	C	2003	4/4	0.83	0.20	19,19,20,21	0
5	ACT	A	2003	4/4	0.86	0.14	19,20,20,21	0
4	NI	B	1003	1/1	0.93	0.08	42,42,42,42	0
5	ACT	B	2002	4/4	0.96	0.11	8,11,11,12	0
4	NI	C	1003	1/1	0.96	0.07	23,23,23,23	0
4	NI	D	1003	1/1	0.97	0.08	37,37,37,37	0
4	NI	A	1003	1/1	0.98	0.05	29,29,29,29	0
4	NI	D	1002	1/1	0.99	0.04	19,19,19,19	0
4	NI	B	1002	1/1	0.99	0.03	16,16,16,16	0
4	NI	A	1002	1/1	0.99	0.02	15,15,15,15	0
4	NI	C	1001	1/1	0.99	0.02	27,27,27,27	0
4	NI	A	1001	1/1	0.99	0.03	20,20,20,20	0
4	NI	D	1001	1/1	0.99	0.04	25,25,25,25	0
4	NI	B	1001	1/1	1.00	0.03	16,16,16,16	0
4	NI	C	1002	1/1	1.00	0.02	19,19,19,19	0

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

There are no such residues in this entry.