



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:39 AM GMT

PDB ID : 2NRA
Title : Crystal structure of Pi initiator protein in complex with iteron DNA
Authors : Swan, M.K.; Bastia, D.; Davies, C.
Deposited on : 2006-11-01
Resolution : 3.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

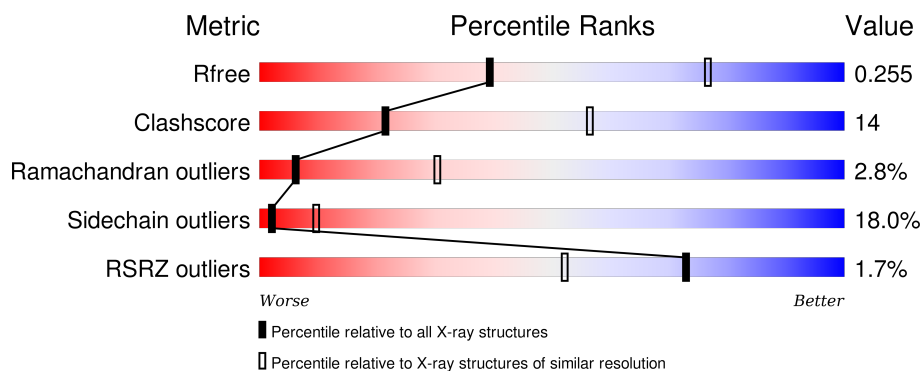
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	A	23	
2	B	23	
3	C	276	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2936 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 5'-D(*GP*AP*AP*CP*AP*TP*GP*AP*GP*AP*GP*C
P*TP*TP*AP*GP*TP*AP*CP*GP*TP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	23	Total	C	N	O	P	0	0	0
			472	226	89	135	22			

- Molecule 2 is a DNA chain called 5'-D(*GP*AP*CP*GP*TP*AP*CP*TP*AP*AP*GP*C
P*TP*CP*TP*CP*AP*TP*GP*TP*TP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	23	Total	C	N	O	P	0	0	0
			464	224	79	139	22			

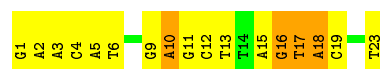
- Molecule 3 is a protein called PI protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	252	Total	C	N	O	S	0	0	0
			2000	1290	336	372	2			

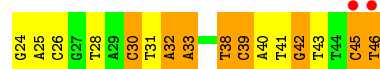
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	42	LEU	PRO	ENGINEERED	UNP P03067
C	106	LEU	PRO	ENGINEERED	UNP P03067
C	107	SER	PHE	ENGINEERED	UNP P03067
C	113	SER	PRO	ENGINEERED	UNP P03067

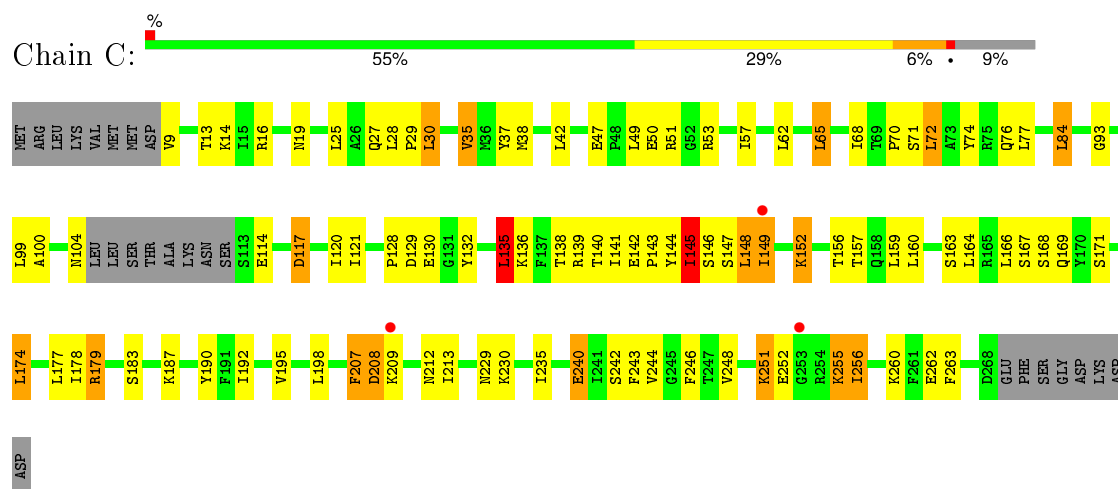
- Molecule 1: 5'-D(*GP*AP*AP*CP*AP*TP*GP*AP*GP*AP*GP*CP*TP*TP*AP*GP*TP*AP*CP*GP*TP*CP*T)-3'



- Molecule 2: 5'-D(*GP*AP*CP*GP*TP*AP*CP*TP*AP*AP*GP*CP*TP*CP*TP*CP*AP*T
P*GP*TP*TP*CP*T)-3'



- Molecule 3: PI protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	125.90Å 125.90Å 138.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.10 – 3.10 35.15 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.10-3.10) 99.5 (35.15-3.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.267 0.214 , 0.255	Depositor DCC
R_{free} test set	593 reflections (5.13%)	DCC
Wilson B-factor (Å ²)	104.4	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 89.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 12161 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2936	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	A	0.93	0/530	1.83	18/817 (2.2%)
2	B	0.96	1/518 (0.2%)	1.94	18/797 (2.3%)
3	C	0.69	0/2035	0.80	1/2741 (0.0%)
All	All	0.79	1/3083 (0.0%)	1.31	37/4355 (0.8%)

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
3	C	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	32	DA	C3'-O3'	-5.26	1.37	1.44

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	42	DG	O4'-C1'-N9	11.14	115.80	108.00
2	B	30	DC	O4'-C1'-N1	10.31	115.22	108.00
2	B	46	DT	O4'-C1'-N1	9.85	114.89	108.00
1	A	9	DG	O4'-C1'-N9	9.71	114.80	108.00
1	A	12	DC	O4'-C1'-N1	9.40	114.58	108.00
1	A	12	DC	C1'-O4'-C4'	-9.18	100.92	110.10
2	B	30	DC	C1'-O4'-C4'	-8.90	101.20	110.10
2	B	42	DG	C1'-O4'-C4'	-8.77	101.33	110.10
1	A	13	DT	C6-C5-C7	-8.46	117.82	122.90
1	A	10	DA	O4'-C4'-C3'	-7.34	101.56	104.50
1	A	18	DA	P-O3'-C3'	7.06	128.17	119.70
2	B	46	DT	C1'-O4'-C4'	-6.80	103.30	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	28	DT	O4'-C1'-N1	6.55	112.58	108.00
1	A	11	DG	P-O3'-C3'	6.41	127.39	119.70
1	A	12	DC	P-O3'-C3'	6.35	127.32	119.70
2	B	40	DA	P-O3'-C3'	6.32	127.28	119.70
2	B	33	DA	P-O3'-C3'	6.31	127.27	119.70
1	A	23	DT	O4'-C1'-N1	6.29	112.41	108.00
1	A	1	DG	P-O3'-C3'	6.01	126.91	119.70
2	B	42	DG	O4'-C4'-C3'	-5.92	102.13	104.50
1	A	9	DG	P-O3'-C3'	5.92	126.80	119.70
1	A	16	DG	O4'-C1'-N9	5.86	112.10	108.00
2	B	28	DT	C1'-O4'-C4'	-5.83	104.27	110.10
2	B	38	DT	O4'-C1'-N1	5.67	111.97	108.00
1	A	12	DC	O4'-C1'-C2'	-5.53	101.48	105.90
2	B	28	DT	C4-C5-C7	5.53	122.31	119.00
1	A	19	DC	O4'-C1'-N1	5.45	111.82	108.00
2	B	39	DC	P-O3'-C3'	5.43	126.21	119.70
2	B	28	DT	N3-C2-O2	-5.42	119.05	122.30
1	A	16	DG	C1'-O4'-C4'	-5.39	104.71	110.10
1	A	11	DG	O4'-C1'-N9	-5.34	104.26	108.00
2	B	24	DG	C4-C5-N7	5.26	112.91	110.80
1	A	17	DT	N3-C4-O4	5.26	123.06	119.90
2	B	24	DG	P-O3'-C3'	5.20	125.94	119.70
1	A	10	DA	P-O3'-C3'	5.19	125.92	119.70
3	C	135	LEU	CA-CB-CG	5.13	127.09	115.30
2	B	45	DC	O4'-C1'-N1	5.09	111.56	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	114	GLU	Peptide
3	C	146	SER	Peptide

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	A	472	0	261	10	0
2	B	464	0	263	11	0
3	C	2000	0	2021	59	0
All	All	2936	0	2545	77	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 14.

All (77) 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)
1:A:5:DA:H2''	1:A:6:DT:H5''	1.32	1.09
1:A:5:DA:H2''	1:A:6:DT:C5'	1.98	0.92
3:C:72:LEU:HD22	3:C:76:GLN:HG3	1.55	0.87
3:C:120:ILE:HG22	3:C:121:ILE:HD12	1.62	0.80
3:C:207:PHE:O	3:C:208:ASP:HB2	1.82	0.78
1:A:5:DA:C2'	1:A:6:DT:H5''	2.14	0.78
3:C:30:LEU:CD1	3:C:167:SER:HA	2.15	0.76
3:C:252:GLU:HB3	3:C:255:LYS:O	1.88	0.74
2:B:26:DC:OP1	3:C:128:PRO:O	2.08	0.71
1:A:17:DT:H2''	1:A:18:DA:H5'	1.71	0.71
3:C:16:ARG:HH22	3:C:149:ILE:HG13	1.56	0.71
3:C:179:ARG:CG	3:C:179:ARG:HH11	2.04	0.70
3:C:138:THR:O	3:C:141:ILE:HG22	1.91	0.70
3:C:152:LYS:NZ	3:C:183:SER:O	2.25	0.66
3:C:248:VAL:HG11	3:C:256:ILE:HD11	1.77	0.66
3:C:207:PHE:O	3:C:208:ASP:CB	2.46	0.63
3:C:140:THR:O	3:C:143:PRO:HD2	1.99	0.62
2:B:45:DC:H2''	2:B:46:DT:C2	2.36	0.61
3:C:179:ARG:HH11	3:C:179:ARG:HG3	1.64	0.61
3:C:144:TYR:C	3:C:145:ILE:HG13	2.23	0.59
3:C:248:VAL:CG1	3:C:256:ILE:HD11	2.33	0.58
2:B:41:DT:H2''	2:B:42:DG:OP2	2.05	0.57
3:C:120:ILE:CG2	3:C:121:ILE:HD12	2.32	0.56
3:C:49:LEU:HD12	3:C:142:GLU:HG2	1.89	0.55
3:C:30:LEU:HD11	3:C:167:SER:HA	1.89	0.55
3:C:19:ASN:ND2	3:C:156:THR:OG1	2.41	0.53
3:C:57:ILE:O	3:C:132:TYR:HB2	2.09	0.53
3:C:147:SER:O	3:C:148:LEU:C	2.47	0.53
2:B:25:DA:H2''	2:B:26:DC:O5'	2.09	0.52
1:A:2:DA:OP2	1:A:2:DA:H2'	2.10	0.51
3:C:246:PHE:HA	3:C:260:LYS:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:DA:C2	1:A:4:DC:C2	2.99	0.51
3:C:16:ARG:NH2	3:C:149:ILE:CG1	2.74	0.51
3:C:157:THR:O	3:C:179:ARG:NH1	2.42	0.51
3:C:16:ARG:HH22	3:C:149:ILE:CG1	2.22	0.49
3:C:135:LEU:C	3:C:135:LEU:HD23	2.32	0.49
2:B:38:DT:C4	2:B:39:DC:N4	2.81	0.49
3:C:166:LEU:HA	3:C:166:LEU:HD23	1.67	0.48
2:B:30:DC:H2''	2:B:31:DT:H5'	1.96	0.48
3:C:84:LEU:HD22	3:C:121:ILE:HD13	1.97	0.47
3:C:35:VAL:HG22	3:C:84:LEU:HD12	1.96	0.47
3:C:16:ARG:NH2	3:C:149:ILE:HG13	2.28	0.47
3:C:243:PHE:O	3:C:263:PHE:HA	2.14	0.47
3:C:104:ASN:HD22	3:C:104:ASN:N	2.12	0.47
3:C:130:GLU:HA	3:C:130:GLU:OE2	2.14	0.47
3:C:179:ARG:HG3	3:C:179:ARG:NH1	2.26	0.47
1:A:15:DA:C2	2:B:32:DA:C2	3.03	0.46
1:A:5:DA:H2''	1:A:6:DT:H5'	1.93	0.46
3:C:229:ASN:O	3:C:230:LYS:C	2.55	0.45
1:A:10:DA:H5'	1:A:10:DA:C8	2.51	0.45
3:C:174:LEU:O	3:C:178:ILE:HG13	2.17	0.45
3:C:14:LYS:HG2	3:C:159:LEU:HD12	1.98	0.45
3:C:190:TYR:HB3	3:C:262:GLU:HG3	1.99	0.45
3:C:168:SER:HB3	3:C:171:SER:HB2	1.99	0.44
3:C:16:ARG:NH2	3:C:149:ILE:HG12	2.33	0.44
3:C:179:ARG:CG	3:C:179:ARG:NH1	2.72	0.43
3:C:70:PRO:O	3:C:71:SER:C	2.56	0.43
1:A:15:DA:C2	1:A:16:DG:C4	3.06	0.43
3:C:100:ALA:O	3:C:104:ASN:ND2	2.52	0.43
3:C:117:ASP:C	3:C:117:ASP:OD1	2.56	0.43
2:B:42:DG:H2''	2:B:43:DT:O5'	2.17	0.43
3:C:68:ILE:HA	3:C:68:ILE:HD13	1.80	0.43
3:C:38:MET:HE3	3:C:65:LEU:HD23	2.00	0.43
3:C:139:ARG:O	3:C:140:THR:C	2.58	0.42
2:B:32:DA:C2	2:B:33:DA:C4	3.07	0.42
3:C:25:LEU:HA	3:C:28:LEU:HD12	2.02	0.42
3:C:37:TYR:CD1	3:C:163:SER:HB3	2.54	0.42
3:C:174:LEU:HB3	3:C:235:ILE:HD11	2.02	0.41
3:C:38:MET:HE3	3:C:164:LEU:HD11	2.01	0.41
3:C:141:ILE:O	3:C:141:ILE:HG13	2.19	0.41
3:C:157:THR:O	3:C:179:ARG:HG2	2.20	0.41
2:B:25:DA:H2'	3:C:74:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:240:GLU:HG3	3:C:240:GLU:H	1.37	0.41
3:C:38:MET:CE	3:C:164:LEU:HD11	2.51	0.40
2:B:31:DT:H2"	2:B:32:DA:OP2	2.22	0.40
3:C:28:LEU:HA	3:C:29:PRO:HD2	1.85	0.40
3:C:9:VAL:O	3:C:13:THR:OG1	2.36	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	C	248 / 276 (90%)	216 (87%)	25 (10%)	7 (3%)	6	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	187	LYS
3	C	208	ASP
3	C	251	LYS
3	C	50	GLU
3	C	93	GLY
3	C	152	LYS
3	C	145	ILE

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	C	211/247 (85%)	173 (82%)	38 (18%)	2 10

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	27	GLN
3	C	30	LEU
3	C	35	VAL
3	C	42	LEU
3	C	47	GLU
3	C	51	ARG
3	C	53	ARG
3	C	62	LEU
3	C	65	LEU
3	C	72	LEU
3	C	77	LEU
3	C	84	LEU
3	C	99	LEU
3	C	117	ASP
3	C	129	ASP
3	C	135	LEU
3	C	136	LYS
3	C	145	ILE
3	C	148	LEU
3	C	149	ILE
3	C	160	LEU
3	C	169	GLN
3	C	174	LEU
3	C	177	LEU
3	C	179	ARG
3	C	192	ILE
3	C	195	VAL
3	C	198	LEU
3	C	207	PHE
3	C	209	LYS
3	C	212	ASN
3	C	213	ILE
3	C	240	GLU
3	C	242	SER
3	C	244	VAL
3	C	251	LYS
3	C	255	LYS
3	C	256	ILE

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

Mol	Chain	Res	Type
3	C	19	ASN
3	C	104	ASN
3	C	181	HIS

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 [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, 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	A	23/23 (100%)	-0.21	0 100 100	68, 83, 95, 130	0
2	B	23/23 (100%)	-0.07	2 (8%) 13 4	62, 85, 126, 147	0
3	C	252/276 (91%)	-0.16	3 (1%) 81 64	59, 78, 96, 107	0
All	All	298/322 (92%)	-0.16	5 (1%) 73 52	59, 79, 100, 147	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	46	DT	3.1
3	C	253	GLY	2.7
3	C	149	ILE	2.6
2	B	45	DC	2.4
3	C	209	LYS	2.1

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 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.