wwPDB X-ray Structure Validation Summary Report (i)

Nov 1, 2023 – 02:32 PM JST

PDB ID	:	5ITR
Title	:	Crystal Structure of Human NEIL1(P2G) bound to duplex DNA containing THF
Authors	:	Zhu, C.; Lu, L.; Zhang, J.; Yue, Z.; Song, J.; Zong, S.; Liu, M.; Stovicek, O.; Gao, Y.; Yi, C.
Deposited on	:	2016-03-17
Resolution	:	2.46 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

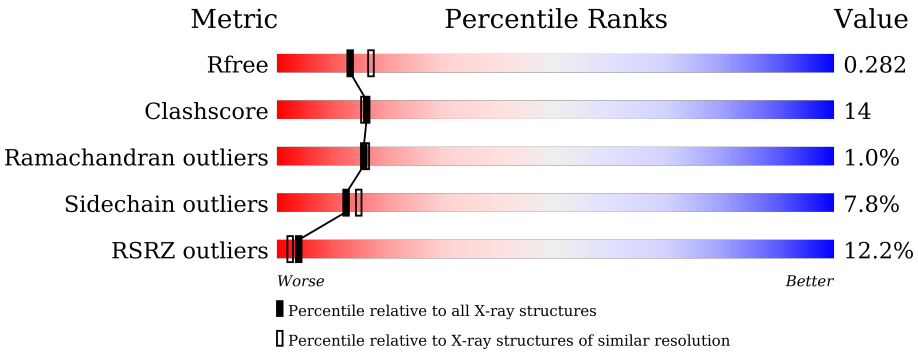
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 <=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	400	3% 52% 12% • 32%
1	B	400	3% 46% 16% • 35%
1	C	400	19% 44% 18% • 36%
2	D	26	8% 77% 23%
2	E	26	65% 31% •
3	F	26	12% 54% 46%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7925 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 protein called Endonuclease 8-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	2	0
			2146	1369	393	374	10			
1	B	261	Total	C	N	O	S	0	0	0
			2073	1324	381	358	10			
1	C	254	Total	C	N	O	S	0	0	0
			2032	1302	371	349	10			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	ARG	LYS	engineered mutation	UNP Q96FI4
A	391	ALA	-	expression tag	UNP Q96FI4
A	392	ALA	-	expression tag	UNP Q96FI4
A	393	LEU	-	expression tag	UNP Q96FI4
A	394	GLY	-	expression tag	UNP Q96FI4
A	395	HIS	-	expression tag	UNP Q96FI4
A	396	HIS	-	expression tag	UNP Q96FI4
A	397	HIS	-	expression tag	UNP Q96FI4
A	398	HIS	-	expression tag	UNP Q96FI4
A	399	HIS	-	expression tag	UNP Q96FI4
A	400	HIS	-	expression tag	UNP Q96FI4
B	242	ARG	LYS	engineered mutation	UNP Q96FI4
B	391	ALA	-	expression tag	UNP Q96FI4
B	392	ALA	-	expression tag	UNP Q96FI4
B	393	LEU	-	expression tag	UNP Q96FI4
B	394	GLY	-	expression tag	UNP Q96FI4
B	395	HIS	-	expression tag	UNP Q96FI4
B	396	HIS	-	expression tag	UNP Q96FI4
B	397	HIS	-	expression tag	UNP Q96FI4
B	398	HIS	-	expression tag	UNP Q96FI4
B	399	HIS	-	expression tag	UNP Q96FI4
B	400	HIS	-	expression tag	UNP Q96FI4
C	242	ARG	LYS	engineered mutation	UNP Q96FI4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	391	ALA	-	expression tag	UNP Q96FI4
C	392	ALA	-	expression tag	UNP Q96FI4
C	393	LEU	-	expression tag	UNP Q96FI4
C	394	GLY	-	expression tag	UNP Q96FI4
C	395	HIS	-	expression tag	UNP Q96FI4
C	396	HIS	-	expression tag	UNP Q96FI4
C	397	HIS	-	expression tag	UNP Q96FI4
C	398	HIS	-	expression tag	UNP Q96FI4
C	399	HIS	-	expression tag	UNP Q96FI4
C	400	HIS	-	expression tag	UNP Q96FI4

- Molecule 2 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	26	Total	C	N	O	P	0	0	0
			516	247	94	151	24			
2	E	26	Total	C	N	O	P	0	0	0
			516	247	94	151	24			

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	26	Total	C	N	O	P	0	0	0
			517	247	94	152	24			

- Molecule 4 is water.

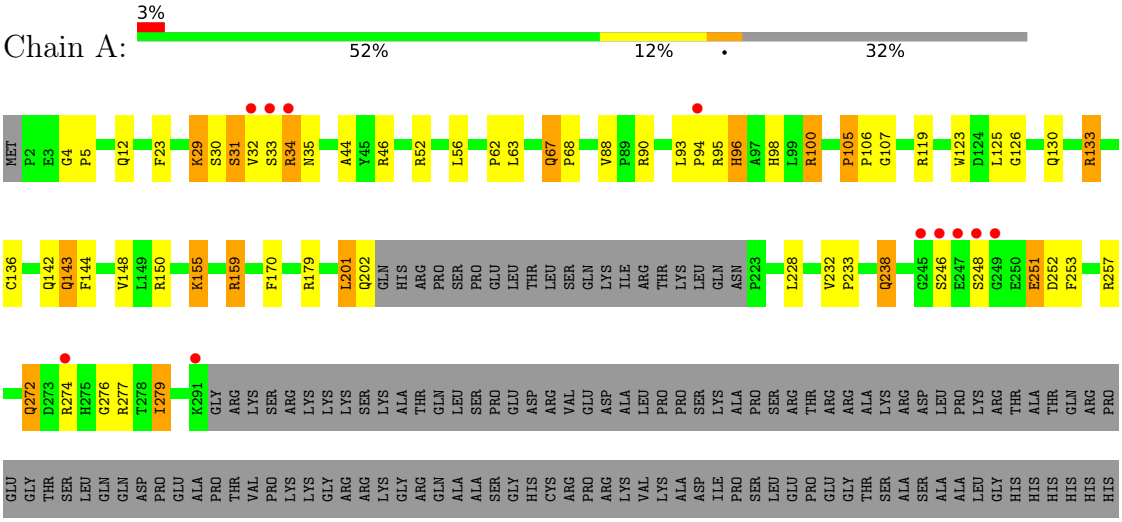
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	B	45	Total	O	0	0
			45	45		
4	C	4	Total	O	0	0
			4	4		
4	D	9	Total	O	0	0
			9	9		
4	E	8	Total	O	0	0
			8	8		

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.

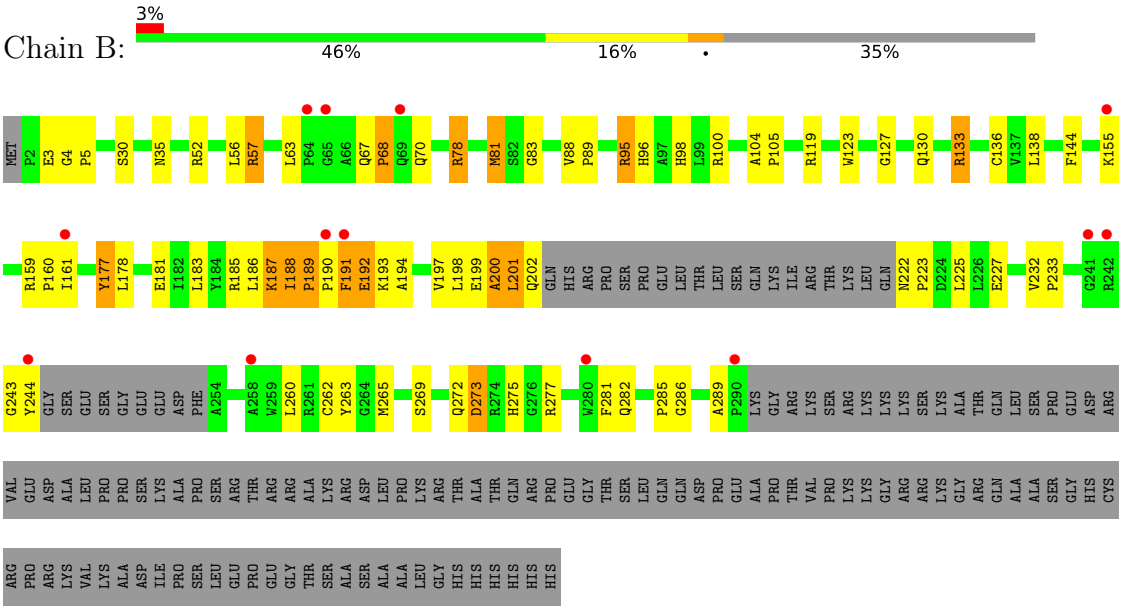
• Molecule 1: Endonuclease 8-like 1

Chain A:



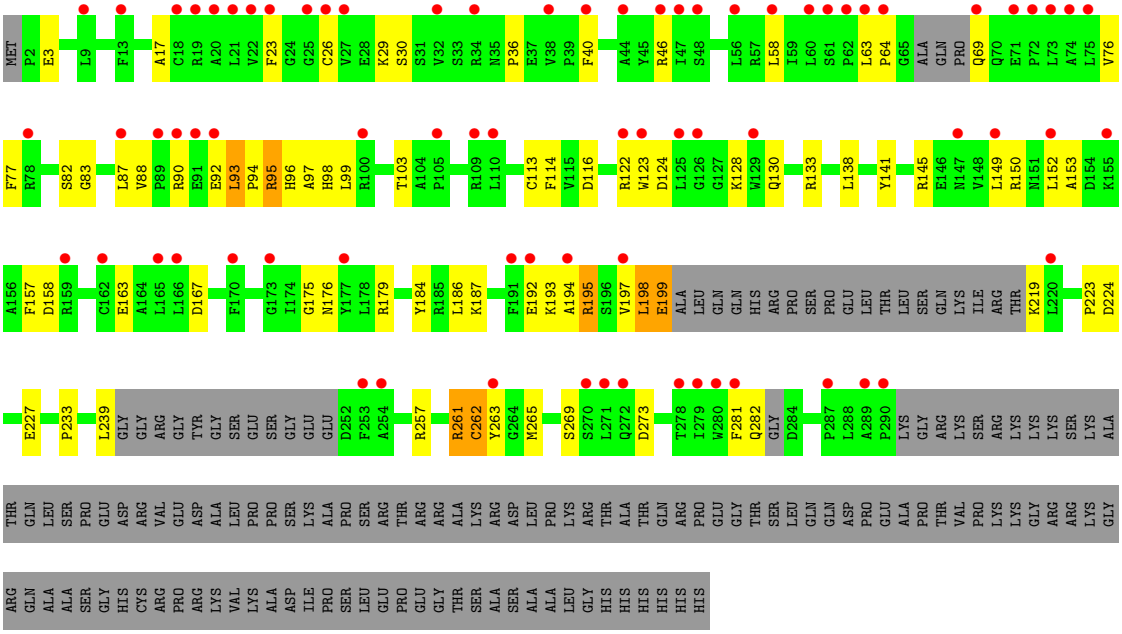
• Molecule 1: Endonuclease 8-like 1

Chain B:

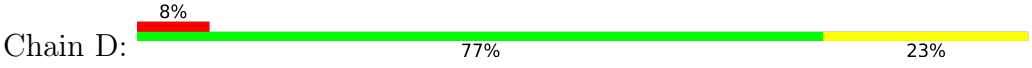


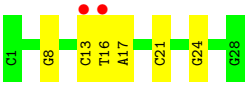
• Molecule 1: Endonuclease 8-like 1

Chain C:

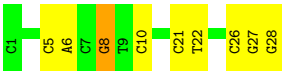


- Molecule 2: DNA (26-MER)

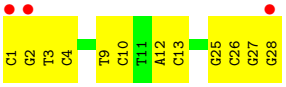




- Molecule 2: DNA (26-MER)



- Molecule 3: DNA (26-MER)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.31Å 109.04Å 169.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.75 – 2.46 44.81 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.4 (91.75-2.46) 99.4 (44.81-2.46)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.211 , 0.263 0.242 , 0.282	Depositor DCC
R_{free} test set	2488 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7925	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	A	1.01	0/2211	1.01	8/2989 (0.3%)
1	B	0.94	2/2129 (0.1%)	1.01	10/2879 (0.3%)
1	C	0.49	0/2085	0.70	1/2816 (0.0%)
2	D	0.53	1/577 (0.2%)	0.83	0/886
2	E	0.56	1/577 (0.2%)	0.97	2/886 (0.2%)
3	F	0.41	0/578	0.76	0/888
All	All	0.79	4/8157 (0.0%)	0.91	21/11344 (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
1	A	0	2
1	B	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	21	DC	O3'-P	-5.36	1.54	1.61
2	E	8	DG	O3'-P	5.11	1.67	1.61
1	B	83	GLY	C-O	-5.11	1.15	1.23
1	B	189	PRO	N-CD	5.08	1.54	1.47

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	133	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	B	57	ARG	NE-CZ-NH2	-8.81	115.90	120.30
2	E	8	DG	O5'-P-OP1	-8.30	98.23	105.70
1	A	133	ARG	NE-CZ-NH2	-8.15	116.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	179	ARG	NE-CZ-NH1	6.85	123.72	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67	GLN	Peptide,Mainchain
1	B	67	GLN	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	2146	0	2109	81	0
1	B	2073	0	2055	66	0
1	C	2032	0	2016	53	0
2	D	516	0	290	5	0
2	E	516	0	290	6	0
3	F	517	0	290	10	0
4	A	59	0	0	1	2
4	B	45	0	0	1	2
4	C	4	0	0	0	0
4	D	9	0	0	1	0
4	E	8	0	0	1	0
All	All	7925	0	7050	215	2

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.

The worst 5 of 215 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:B:191:PHE:CE2	1:B:289:ALA:HB2	1.16	1.58
1:B:191:PHE:CE2	1:B:289:ALA:CB	1.97	1.47
1:B:191:PHE:CZ	1:B:289:ALA:CB	2.10	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:PHE:CZ	1:B:289:ALA:HB2	1.75	1.16
1:B:191:PHE:CD2	1:B:289:ALA:HB2	1.81	1.15

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:551:HOH:O	4:B:525:HOH:O[3_555]	1.81	0.39
4:A:558:HOH:O	4:B:537:HOH:O[3_555]	1.99	0.21

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	
1	A	268/400 (67%)	251 (94%)	15 (6%)	2 (1%)	22	25
1	B	255/400 (64%)	231 (91%)	22 (9%)	2 (1%)	19	22
1	C	244/400 (61%)	215 (88%)	25 (10%)	4 (2%)	9	8
All	All	767/1200 (64%)	697 (91%)	62 (8%)	8 (1%)	15	16

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	PRO
1	B	68	PRO
1	B	200	ALA
1	C	36	PRO
1	C	97	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	
1	A	222/335 (66%)	203 (91%)	19 (9%)	10	11
1	B	216/335 (64%)	201 (93%)	15 (7%)	15	18
1	C	214/335 (64%)	197 (92%)	17 (8%)	12	14
All	All	652/1005 (65%)	601 (92%)	51 (8%)	12	15

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	192	GLU
1	C	69	GLN
1	C	261	ARG
1	B	201	LEU
1	B	273	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	130	GLN
1	B	143	GLN
1	C	282	GLN
1	C	139	GLN
1	C	151	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 monosaccharides 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^{th} 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	270/400 (67%)	0.44	11 (4%) 37 34	13, 31, 61, 85	0
1	B	261/400 (65%)	0.59	13 (4%) 28 26	19, 41, 74, 124	0
1	C	254/400 (63%)	1.65	76 (29%) 0 0	48, 88, 121, 149	0
2	D	26/26 (100%)	0.10	2 (7%) 13 10	34, 67, 110, 118	0
2	E	26/26 (100%)	0.10	0 100 100	29, 64, 79, 85	0
3	F	26/26 (100%)	0.61	3 (11%) 4 3	68, 98, 111, 116	0
All	All	863/1278 (67%)	0.82	105 (12%) 4 2	13, 50, 110, 149	0

The worst 5 of 105 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	75	LEU	13.0
1	B	191	PHE	8.9
1	B	242	ARG	8.7
1	C	23	PHE	8.5
1	C	110	LEU	8.0

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

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.