Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:49 AM GMT

PDB ID	:	3G6T
Title	:	GR gamma DNA-binding domain:FKBP5 16bp complex-34
Authors	:	Pufall, M.A.; Yamamoto, K.R.; Meijsing, S.H.
Deposited on	:	2009-02-08
Resolution	:	1.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

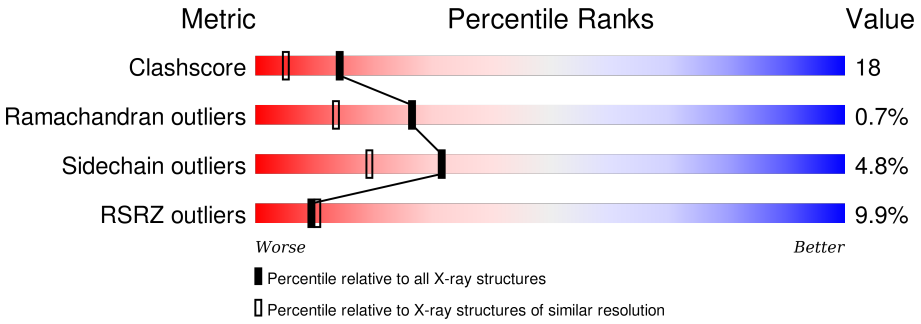
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 <=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	91	8% 60% 20% 5% 14%
1	B	91	12% 63% 14% • 21%
2	D	16	31% 63% 6%
3	C	16	31% 44% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ZN	A	528	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1915 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 Glucocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	78	Total	C	N	O	S	0	0	0
			603	366	120	105	12			
1	B	72	Total	C	N	O	S	0	0	0
			555	338	108	97	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	GLY	-	EXPRESSION TAG	UNP P06536
A	437	SER	-	EXPRESSION TAG	UNP P06536
A	438	HIS	-	EXPRESSION TAG	UNP P06536
A	439	MET	-	EXPRESSION TAG	UNP P06536
A	471	ARG	-	INSERTION	UNP P06536
B	436	GLY	-	EXPRESSION TAG	UNP P06536
B	437	SER	-	EXPRESSION TAG	UNP P06536
B	438	HIS	-	EXPRESSION TAG	UNP P06536
B	439	MET	-	EXPRESSION TAG	UNP P06536
B	471	ARG	-	INSERTION	UNP P06536

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	16	Total	C	N	O	P	0	0	0
			320	155	55	95	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	16	Total	C	N	O	P	0	0	0
			330	158	64	93	15			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Zn 2 2	0	0
4	A	2	Total Zn 2 2	0	0

- Molecule 5 is water.

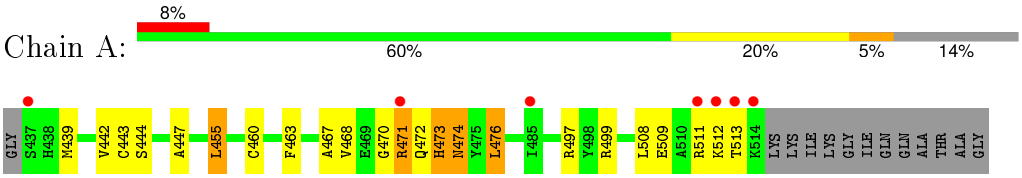
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	43	Total O 43 43	0	0
5	B	32	Total O 32 32	0	0
5	D	18	Total O 18 18	0	0
5	C	10	Total O 10 10	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

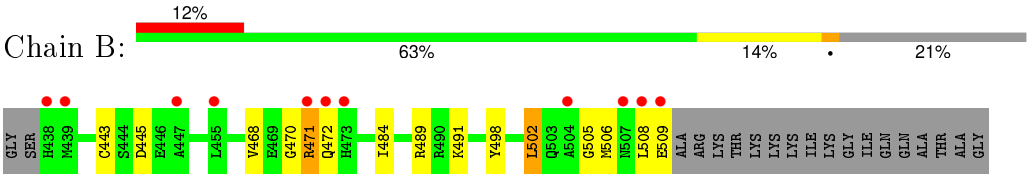
• Molecule 1: Glucocorticoid receptor

Chain A:



• Molecule 1: Glucocorticoid receptor

Chain B:



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

Chain D:

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

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	115.69Å 39.72Å 95.23Å 90.00° 122.79° 90.00°	Depositor
Resolution (Å)	31.09 – 1.90 31.09 – 1.90	Depositor EDS
% Data completeness (in resolution range)	84.4 (31.09-1.90) 84.5 (31.09-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.179 , 0.214 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 68.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 26430 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	1915	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 7.42% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN

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	1.10	4/611 (0.7%)	0.98	2/814 (0.2%)
1	B	0.61	0/562	0.65	0/749
2	D	1.30	2/357 (0.6%)	2.00	15/548 (2.7%)
3	C	1.39	3/371 (0.8%)	2.54	27/572 (4.7%)
All	All	1.09	9/1901 (0.5%)	1.61	44/2683 (1.6%)

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	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	DA	N9-C4	-8.76	1.32	1.37
3	C	1	DA	C2-N3	-6.33	1.27	1.33
2	D	15	DC	C3'-O3'	-6.11	1.36	1.44
1	A	499	ARG	CG-CD	5.64	1.66	1.51
2	D	13	DT	O3'-P	-5.42	1.54	1.61
1	A	442	VAL	CB-CG1	5.40	1.64	1.52
3	C	1	DA	C5-C6	-5.30	1.36	1.41
1	A	463	PHE	CD2-CE2	5.24	1.49	1.39
1	A	460	CYS	CB-SG	5.20	1.91	1.82

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	DA	C2-N3-C4	-16.64	102.28	110.60
3	C	1	DA	C5-C6-N1	-11.73	111.84	117.70
3	C	9	DG	N1-C6-O6	11.66	126.89	119.90
3	C	1	DA	N3-C4-C5	11.63	134.94	126.80
3	C	1	DA	C5-N7-C8	-10.66	98.57	103.90
3	C	9	DG	O4'-C1'-N9	-10.45	100.68	108.00
3	C	1	DA	N3-C4-N9	-10.31	119.15	127.40
3	C	1	DA	C6-N1-C2	9.96	124.57	118.60
3	C	9	DG	C5-C6-O6	-9.88	122.67	128.60
3	C	5	DA	O4'-C1'-N9	8.13	113.69	108.00
3	C	9	DG	C4-C5-N7	8.07	114.03	110.80
2	D	11	DT	N3-C4-O4	8.02	124.71	119.90
3	C	9	DG	C6-C5-N7	-7.99	125.60	130.40
3	C	9	DG	N9-C4-C5	-7.72	102.31	105.40
2	D	14	DT	C6-C5-C7	-6.86	118.78	122.90
2	D	9	DC	O4'-C1'-N1	6.56	112.59	108.00
3	C	1	DA	N7-C8-N9	6.55	117.08	113.80
3	C	1	DA	C4-C5-N7	6.53	113.97	110.70
2	D	11	DT	C5-C4-O4	-6.41	120.42	124.90
3	C	14	DT	O4'-C1'-N1	-6.33	103.57	108.00
3	C	9	DG	C1'-O4'-C4'	-6.24	103.86	110.10
2	D	14	DT	C4-C5-C7	6.13	122.68	119.00
2	D	10	DC	N3-C2-O2	-6.07	117.65	121.90
2	D	15	DC	O5'-P-OP2	-5.98	100.31	105.70
2	D	5	DA	O4'-C1'-N9	-5.93	103.85	108.00
3	C	1	DA	N9-C1'-C2'	-5.91	101.36	112.60
1	A	474	ASN	N-CA-C	5.87	126.84	111.00
2	D	14	DT	O4'-C1'-N1	-5.84	103.91	108.00
2	D	12	DG	C2-N3-C4	5.83	114.81	111.90
3	C	9	DG	O4'-C1'-C2'	-5.80	101.26	105.90
1	A	497	ARG	NE-CZ-NH1	-5.53	117.53	120.30
3	C	3	DG	C1'-O4'-C4'	-5.51	104.59	110.10
3	C	1	DA	C5-C6-N6	5.48	128.08	123.70
3	C	5	DA	C3'-C2'-C1'	-5.46	95.95	102.50
2	D	11	DT	N3-C2-O2	5.45	125.57	122.30
2	D	11	DT	C4-C5-C7	5.43	122.26	119.00
2	D	10	DC	C6-N1-C2	-5.33	118.17	120.30
2	D	14	DT	P-O3'-C3'	5.26	126.01	119.70
3	C	1	DA	C4'-C3'-O3'	5.25	122.81	109.70
3	C	11	DT	C4-C5-C7	5.22	122.13	119.00
3	C	2	DA	C5-C6-N6	5.15	127.82	123.70
2	D	11	DT	C5-C6-N1	5.11	126.77	123.70
3	C	4	DA	N1-C2-N3	-5.01	126.80	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1	DA	O4'-C1'-C2'	5.00	109.90	105.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	473	HIS	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	A	603	0	592	28	0
1	B	555	0	542	14	0
2	D	320	0	183	7	0
3	C	330	0	182	17	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	43	0	0	1	0
5	B	32	0	0	0	0
5	C	10	0	0	1	0
5	D	18	0	0	0	0
All	All	1915	0	1499	54	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 18.

All (54) 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:1:DA:HO5'	3:C:1:DA:H8	1.03	1.01
1:B:470:GLY:HA3	1:B:471:ARG:HB2	1.38	1.00
1:A:471:ARG:HB3	1:A:472:GLN:HA	1.49	0.94
1:B:484:ILE:HG21	1:B:489:ARG:HH11	1.41	0.86
3:C:15:DC:H2"	3:C:16:DT:C5'	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:GLY:CA	1:B:471:ARG:HB2	2.13	0.75
1:A:471:ARG:CB	1:A:472:GLN:HA	2.16	0.75
3:C:15:DC:H2"	3:C:16:DT:H5'	1.69	0.73
3:C:15:DC:H2"	3:C:16:DT:O5'	1.87	0.72
2:D:16:DT:OP1	2:D:16:DT:H3'	1.88	0.72
1:A:447:ALA:CB	1:A:455:LEU:HD13	2.26	0.64
1:B:472:GLN:HG3	1:B:498:TYR:CE2	2.33	0.63
1:A:472:GLN:O	1:A:473:HIS:HB2	1.97	0.63
1:A:476:LEU:HD23	1:B:489:ARG:HH21	1.64	0.63
1:A:511:ARG:HD2	3:C:2:DA:C5'	2.31	0.60
1:A:472:GLN:CG	1:A:474:ASN:ND2	2.65	0.59
1:B:443:CYS:SG	1:B:445:ASP:HB2	2.42	0.59
3:C:1:DA:N6	5:C:84:HOH:O	2.37	0.57
1:A:513:THR:HG22	1:A:513:THR:O	2.04	0.57
3:C:15:DC:C2'	3:C:16:DT:H5'	2.35	0.57
2:D:9:DC:N4	3:C:9:DG:H1	2.02	0.57
1:B:470:GLY:HA3	1:B:471:ARG:CB	2.21	0.56
1:A:472:GLN:HG2	1:A:474:ASN:ND2	2.21	0.55
1:A:476:LEU:CD2	1:B:489:ARG:HH21	2.21	0.54
1:A:476:LEU:HD23	1:B:489:ARG:NH2	2.23	0.53
1:A:472:GLN:HG2	1:A:474:ASN:CG	2.29	0.52
1:A:470:GLY:O	1:A:471:ARG:HB2	2.10	0.52
1:B:468:VAL:HG11	1:B:508:LEU:HD21	1.92	0.51
1:A:467:ALA:O	1:A:471:ARG:CG	2.60	0.49
1:A:511:ARG:HD2	3:C:2:DA:H5"	1.94	0.49
2:D:1:DT:H2"	2:D:2:DA:C8	2.48	0.49
1:A:467:ALA:O	1:A:471:ARG:HG2	2.12	0.49
1:A:471:ARG:HB3	1:A:472:GLN:CA	2.34	0.48
2:D:16:DT:OP1	2:D:16:DT:C3'	2.60	0.48
2:D:9:DC:N4	3:C:9:DG:N1	2.61	0.47
3:C:9:DG:H2"	3:C:10:DG:H8	1.79	0.47
3:C:9:DG:H2"	3:C:10:DG:C8	2.50	0.46
1:A:509:GLU:OE1	1:A:512:LYS:HD2	2.16	0.46
1:A:511:ARG:HD2	3:C:2:DA:H5'	1.96	0.45
1:A:443:CYS:O	1:A:444:SER:HB2	2.17	0.45
1:A:509:GLU:OE1	1:A:512:LYS:HB2	2.17	0.45
1:A:513:THR:CG2	1:A:513:THR:O	2.64	0.44
2:D:9:DC:N3	3:C:9:DG:C2	2.85	0.44
1:A:468:VAL:HG21	1:A:508:LEU:HD13	2.00	0.43
1:A:472:GLN:HB2	5:A:101:HOH:O	2.18	0.43
1:A:447:ALA:HB1	1:A:455:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LEU:HD22	1:A:455:LEU:HA	1.88	0.42
1:B:491:LYS:HG3	3:C:11:DT:H5"	2.01	0.42
1:B:502:LEU:HD12	1:B:502:LEU:HA	1.85	0.42
2:D:9:DC:N3	3:C:9:DG:N2	2.67	0.41
3:C:1:DA:H2'	3:C:1:DA:O5'	2.21	0.41
1:A:476:LEU:CD2	1:B:489:ARG:NH2	2.83	0.41
1:A:472:GLN:O	1:A:474:ASN:OD1	2.40	0.40
1:B:505:GLY:O	1:B:506:MET:C	2.59	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
1	A	76/91 (84%)	69 (91%)	7 (9%)	0	100 100
1	B	70/91 (77%)	64 (91%)	5 (7%)	1 (1%)	14 4
All	All	146/182 (80%)	133 (91%)	12 (8%)	1 (1%)	26 14

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	471	ARG

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	65/74 (88%)	61 (94%)	4 (6%)	23 11
1	B	60/74 (81%)	58 (97%)	2 (3%)	45 34
All	All	125/148 (84%)	119 (95%)	6 (5%)	31 19

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	439	MET
1	A	455	LEU
1	A	471	ARG
1	A	476	LEU
1	B	502	LEU
1	B	509	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	507	ASN
1	B	473	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)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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

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	78/91 (85%)	0.65	7 (8%) 12 13	31, 43, 128, 150	0
1	B	72/91 (79%)	0.85	11 (15%) 3 3	32, 79, 127, 202	0
2	D	16/16 (100%)	-0.14	0 100 100	45, 94, 125, 128	0
3	C	16/16 (100%)	0.01	0 100 100	58, 73, 123, 136	0
All	All	182/214 (85%)	0.61	18 (9%) 9 10	31, 64, 128, 202	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	THR	7.0
1	B	447	ALA	5.5
1	B	439	MET	5.0
1	A	514	LYS	4.7
1	A	511	ARG	4.1
1	B	507	ASN	3.6
1	B	438	HIS	3.4
1	A	512	LYS	3.4
1	B	508	LEU	3.3
1	B	455	LEU	3.0
1	B	473	HIS	2.9
1	A	437	SER	2.9
1	B	472	GLN	2.6
1	B	504	ALA	2.5
1	A	485	ILE	2.4
1	A	471	ARG	2.3
1	B	509	GLU	2.3
1	B	471	ARG	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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	ZN	A	528	1/1	1.00	0.13	2.27	35,35,35,35	0
4	ZN	B	528	1/1	0.99	0.12	0.88	38,38,38,38	0
4	ZN	A	527	1/1	1.00	0.12	0.27	39,39,39,39	0
4	ZN	B	527	1/1	1.00	0.08	-1.61	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.