wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 03:44 PM EDT

PDB ID	:	5CC1
Title	:	S425G Glucocorticoid receptor DNA binding domain - (+)GRE complex
Authors	:	Hudson, W.H.; Weikum, E.A.; Ortlund, E.A.
Deposited on	:	2015-07-01
Resolution	:	2.30 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 (i)) were used in the production of this report:

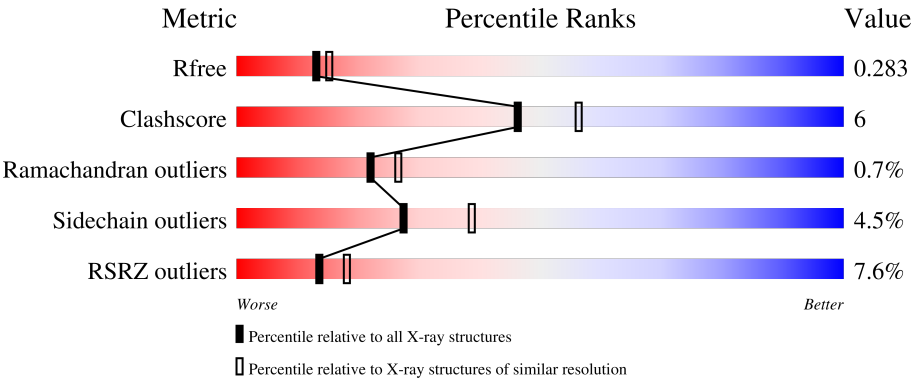
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	114	5% 57% 8% • 34%
1	B	114	7% 49% 11% • • 36%
1	W	114	4% 60% 5% • 34%
1	X	114	8% 51% 11% •• 36%
2	C	18	83% 17%

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Mol	Chain	Length	Quality of chain
2	Z	18	83% 17%
3	D	18	72% 28%
3	Y	18	83% 17%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3756 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	75	Total	C	N	O	S	0	0	0
			576	354	112	99	11			
1	B	73	Total	C	N	O	S	0	0	0
			558	343	107	97	11			
1	W	75	Total	C	N	O	S	0	0	0
			576	354	112	99	11			
1	X	73	Total	C	N	O	S	0	0	0
			558	343	107	97	11			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	393	MET	-	initiating methionine	UNP P04150
A	394	HIS	-	expression tag	UNP P04150
A	395	HIS	-	expression tag	UNP P04150
A	396	HIS	-	expression tag	UNP P04150
A	397	HIS	-	expression tag	UNP P04150
A	398	HIS	-	expression tag	UNP P04150
A	399	HIS	-	expression tag	UNP P04150
A	400	SER	-	expression tag	UNP P04150
A	401	SER	-	expression tag	UNP P04150
A	402	GLY	-	expression tag	UNP P04150
A	403	VAL	-	expression tag	UNP P04150
A	404	ASP	-	expression tag	UNP P04150
A	405	LEU	-	expression tag	UNP P04150
A	406	GLY	-	expression tag	UNP P04150
A	407	THR	-	expression tag	UNP P04150
A	408	GLU	-	expression tag	UNP P04150
A	409	ASN	-	expression tag	UNP P04150
A	410	LEU	-	expression tag	UNP P04150
A	411	TYR	-	expression tag	UNP P04150
A	412	PHE	-	expression tag	UNP P04150
A	413	GLN	-	expression tag	UNP P04150

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Chain	Residue	Modelled	Actual	Comment	Reference
A	414	SER	-	expression tag	UNP P04150
A	415	ASN	-	expression tag	UNP P04150
A	416	ALA	-	expression tag	UNP P04150
A	425	GLY	SER	engineered mutation	UNP P04150
B	393	MET	-	initiating methionine	UNP P04150
B	394	HIS	-	expression tag	UNP P04150
B	395	HIS	-	expression tag	UNP P04150
B	396	HIS	-	expression tag	UNP P04150
B	397	HIS	-	expression tag	UNP P04150
B	398	HIS	-	expression tag	UNP P04150
B	399	HIS	-	expression tag	UNP P04150
B	400	SER	-	expression tag	UNP P04150
B	401	SER	-	expression tag	UNP P04150
B	402	GLY	-	expression tag	UNP P04150
B	403	VAL	-	expression tag	UNP P04150
B	404	ASP	-	expression tag	UNP P04150
B	405	LEU	-	expression tag	UNP P04150
B	406	GLY	-	expression tag	UNP P04150
B	407	THR	-	expression tag	UNP P04150
B	408	GLU	-	expression tag	UNP P04150
B	409	ASN	-	expression tag	UNP P04150
B	410	LEU	-	expression tag	UNP P04150
B	411	TYR	-	expression tag	UNP P04150
B	412	PHE	-	expression tag	UNP P04150
B	413	GLN	-	expression tag	UNP P04150
B	414	SER	-	expression tag	UNP P04150
B	415	ASN	-	expression tag	UNP P04150
B	416	ALA	-	expression tag	UNP P04150
B	425	GLY	SER	engineered mutation	UNP P04150
W	393	MET	-	initiating methionine	UNP P04150
W	394	HIS	-	expression tag	UNP P04150
W	395	HIS	-	expression tag	UNP P04150
W	396	HIS	-	expression tag	UNP P04150
W	397	HIS	-	expression tag	UNP P04150
W	398	HIS	-	expression tag	UNP P04150
W	399	HIS	-	expression tag	UNP P04150
W	400	SER	-	expression tag	UNP P04150
W	401	SER	-	expression tag	UNP P04150
W	402	GLY	-	expression tag	UNP P04150
W	403	VAL	-	expression tag	UNP P04150
W	404	ASP	-	expression tag	UNP P04150
W	405	LEU	-	expression tag	UNP P04150

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Chain	Residue	Modelled	Actual	Comment	Reference
W	406	GLY	-	expression tag	UNP P04150
W	407	THR	-	expression tag	UNP P04150
W	408	GLU	-	expression tag	UNP P04150
W	409	ASN	-	expression tag	UNP P04150
W	410	LEU	-	expression tag	UNP P04150
W	411	TYR	-	expression tag	UNP P04150
W	412	PHE	-	expression tag	UNP P04150
W	413	GLN	-	expression tag	UNP P04150
W	414	SER	-	expression tag	UNP P04150
W	415	ASN	-	expression tag	UNP P04150
W	416	ALA	-	expression tag	UNP P04150
W	425	GLY	SER	engineered mutation	UNP P04150
X	393	MET	-	initiating methionine	UNP P04150
X	394	HIS	-	expression tag	UNP P04150
X	395	HIS	-	expression tag	UNP P04150
X	396	HIS	-	expression tag	UNP P04150
X	397	HIS	-	expression tag	UNP P04150
X	398	HIS	-	expression tag	UNP P04150
X	399	HIS	-	expression tag	UNP P04150
X	400	SER	-	expression tag	UNP P04150
X	401	SER	-	expression tag	UNP P04150
X	402	GLY	-	expression tag	UNP P04150
X	403	VAL	-	expression tag	UNP P04150
X	404	ASP	-	expression tag	UNP P04150
X	405	LEU	-	expression tag	UNP P04150
X	406	GLY	-	expression tag	UNP P04150
X	407	THR	-	expression tag	UNP P04150
X	408	GLU	-	expression tag	UNP P04150
X	409	ASN	-	expression tag	UNP P04150
X	410	LEU	-	expression tag	UNP P04150
X	411	TYR	-	expression tag	UNP P04150
X	412	PHE	-	expression tag	UNP P04150
X	413	GLN	-	expression tag	UNP P04150
X	414	SER	-	expression tag	UNP P04150
X	415	ASN	-	expression tag	UNP P04150
X	416	ALA	-	expression tag	UNP P04150
X	425	GLY	SER	engineered mutation	UNP P04150

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	18	Total 368	C 176	N 70	O 105	P 17	0	0	0
2	Z	18	Total 368	C 176	N 70	O 105	P 17	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	18	Total 362	C 175	N 62	O 108	P 17	0	0	0
3	Y	18	Total 362	C 175	N 62	O 108	P 17	0	0	0

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

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

- Molecule 5 is water.

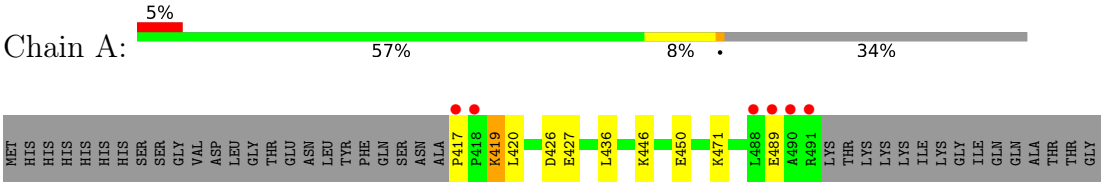
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	O 6	0	0
5	B	3	Total 3	O 3	0	0
5	W	7	Total 7	O 7	0	0
5	X	4	Total 4	O 4	0	0

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.

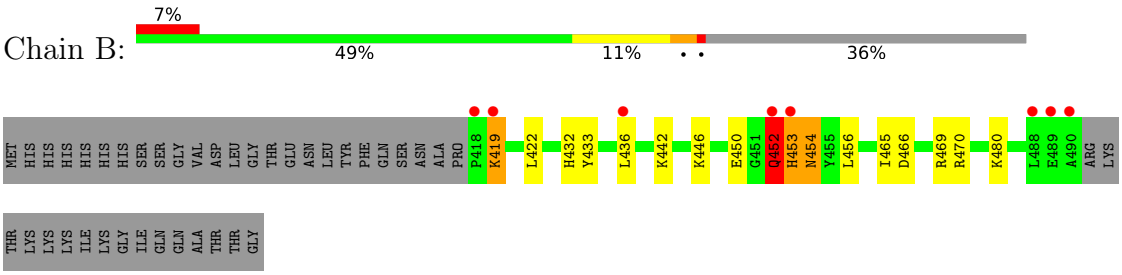
• Molecule 1: Glucocorticoid receptor

Chain A:



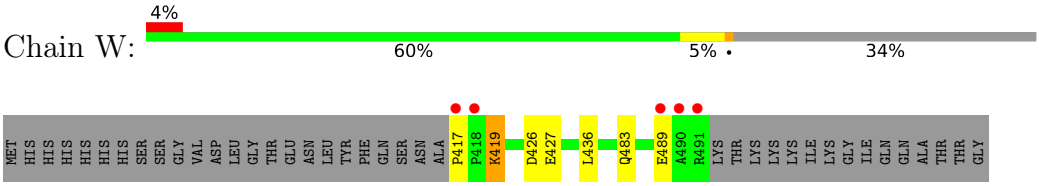
• Molecule 1: Glucocorticoid receptor

Chain B:



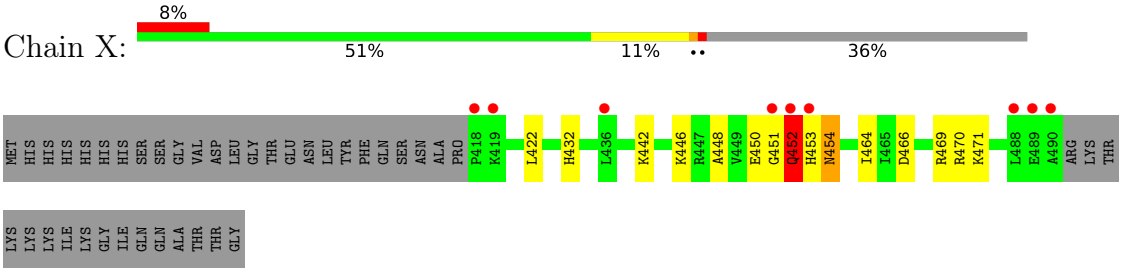
• Molecule 1: Glucocorticoid receptor

Chain W:



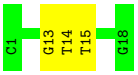
• Molecule 1: Glucocorticoid receptor

Chain X:



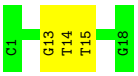
• Molecule 2: DNA (5'-D(*CP*CP*AP*GP*AP*AP*CP*AP*GP*AP*GP*TP*GP*TP*TP*CP*TP*G)-3')

Chain C:



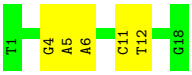
• Molecule 2: DNA (5'-D(*CP*CP*AP*GP*AP*AP*CP*AP*GP*AP*GP*TP*GP*TP*TP*CP*TP*G)-3')

Chain Z:



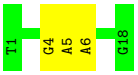
• Molecule 3: DNA (5'-D(*TP*CP*AP*GP*AP*AP*CP*AP*CP*TP*CP*TP*GP*TP*TP*CP*TP*G)-3')

Chain D:



• Molecule 3: DNA (5'-D(*TP*CP*AP*GP*AP*AP*CP*AP*CP*TP*CP*TP*GP*TP*TP*CP*TP*G)-3')

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	176.72Å 39.12Å 132.10Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	32.41 – 2.30 32.41 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.4 (32.41-2.30) 91.5 (32.41-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.245 , 0.279 0.258 , 0.283	Depositor DCC
R_{free} test set	1947 reflections (5.31%)	wwPDB-VP
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3756	wwPDB-VP
Average B, all atoms (Å^2)	70.0	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 99.80 % 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 1.6875e-14. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.59	0/585	0.73	0/781
1	B	0.50	0/566	0.74	0/755
1	W	0.59	0/585	0.70	0/781
1	X	0.52	0/566	0.86	3/755 (0.4%)
2	C	0.78	0/413	0.92	0/636
2	Z	0.77	0/413	0.92	0/636
3	D	0.85	0/404	1.00	0/621
3	Y	0.86	0/404	0.99	0/621
All	All	0.67	0/3936	0.86	3/5586 (0.1%)

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	B	0	1
1	W	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	452	GLN	CA-CB-CG	7.78	130.52	113.40
1	X	452	GLN	CB-CA-C	7.59	125.58	110.40
1	X	452	GLN	CA-C-N	5.28	128.82	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	452	GLN	Peptide
1	W	417	PRO	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	576	0	573	6	0
1	B	558	0	553	13	0
1	W	576	0	573	4	0
1	X	558	0	553	15	0
2	C	368	0	204	2	0
2	Z	368	0	204	2	0
3	D	362	0	206	3	0
3	Y	362	0	206	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	W	2	0	0	0	0
4	X	2	0	0	0	0
5	A	6	0	0	0	0
5	B	3	0	0	0	0
5	W	7	0	0	0	0
5	X	4	0	0	0	0
All	All	3756	0	3072	43	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 6.

The worst 5 of 43 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:419:LYS:HE3	1:B:436:LEU:HD22	1.72	0.70
1:W:419:LYS:HB3	1:W:436:LEU:HD21	1.74	0.68
2:C:14:DT:H2"	2:C:15:DT:H5'	1.77	0.67
2:Z:14:DT:H2"	2:Z:15:DT:H5'	1.77	0.66
1:B:452:GLN:HG3	1:B:453:HIS:CB	2.28	0.64

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	73/114 (64%)	72 (99%)	1 (1%)	0	100	100
1	B	71/114 (62%)	68 (96%)	2 (3%)	1 (1%)	11	11
1	W	73/114 (64%)	72 (99%)	1 (1%)	0	100	100
1	X	71/114 (62%)	64 (90%)	6 (8%)	1 (1%)	11	11
All	All	288/456 (63%)	276 (96%)	10 (4%)	2 (1%)	22	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	452	GLN
1	B	452	GLN

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	62/95 (65%)	58 (94%)	4 (6%)	17	23
1	B	60/95 (63%)	57 (95%)	3 (5%)	24	34
1	W	62/95 (65%)	60 (97%)	2 (3%)	39	54
1	X	60/95 (63%)	58 (97%)	2 (3%)	38	53
All	All	244/380 (64%)	233 (96%)	11 (4%)	27	39

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	419	LYS
1	W	489	GLU
1	X	471	LYS
1	X	454	ASN
1	B	419	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	453	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 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 (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	75/114 (65%)	0.60	6 (8%) 12 16	40, 53, 87, 110	0
1	B	73/114 (64%)	0.84	8 (10%) 5 7	44, 68, 96, 109	0
1	W	75/114 (65%)	0.64	5 (6%) 17 23	40, 53, 89, 110	0
1	X	73/114 (64%)	0.88	9 (12%) 4 6	44, 69, 97, 110	0
2	C	18/18 (100%)	0.16	0 100 100	60, 78, 95, 97	0
2	Z	18/18 (100%)	0.17	0 100 100	60, 78, 95, 98	0
3	D	18/18 (100%)	0.06	0 100 100	65, 82, 98, 101	0
3	Y	18/18 (100%)	0.09	0 100 100	65, 82, 98, 101	0
All	All	368/528 (69%)	0.62	28 (7%) 13 18	40, 65, 97, 110	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	417	PRO	6.1
1	B	452	GLN	5.9
1	A	417	PRO	5.9
1	W	491	ARG	5.8
1	B	490	ALA	5.7

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 (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^{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	B-factors(Å^2)	Q<0.9
4	ZN	A	601	1/1	0.98	0.16	52,52,52,52	0
4	ZN	W	601	1/1	0.98	0.15	52,52,52,52	0
4	ZN	B	602	1/1	0.99	0.15	45,45,45,45	0
4	ZN	B	601	1/1	0.99	0.12	65,65,65,65	0
4	ZN	X	601	1/1	0.99	0.12	65,65,65,65	0
4	ZN	X	602	1/1	0.99	0.15	46,46,46,46	0
4	ZN	A	602	1/1	1.00	0.14	43,43,43,43	0
4	ZN	W	602	1/1	1.00	0.14	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.