wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 06:00 AM EDT

PDB ID	:	6OV0
Title	:	Crystal structure of Csm6 in complex with A4>p by soaking A4>p into Csm6
Authors	:	Jia, N.; Patel, D.J.
Deposited on	:	2019-05-06
Resolution	:	2.80 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:

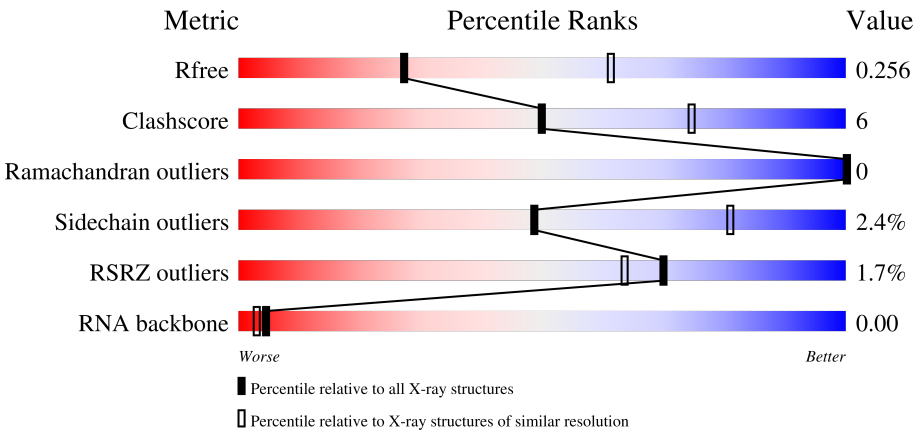
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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	440	2% 90% 9% •
1	B	440	.% 88% 10% •
1	C	440	.% 88% 10% • •
1	D	440	2% 88% 9% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	4	25% 50% 25%
2	F	4	25% 25% 25% 25%
2	G	4	25% 25% 25% 25%
2	H	4	25% 50% 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
2	A23	E	4	-	-	X	-
2	A23	G	4	-	-	X	-
2	A23	H	4	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14052 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	433	3450	2220	586	636	8	0	0	0
1	B	432	3440	2214	583	635	8	0	0	0
1	C	433	3450	2220	586	636	8	0	0	0
1	D	432	3440	2214	583	635	8	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP B6YWC3
A	0	GLY	-	expression tag	UNP B6YWC3
A	433	HIS	-	expression tag	UNP B6YWC3
A	434	HIS	-	expression tag	UNP B6YWC3
A	435	HIS	-	expression tag	UNP B6YWC3
A	436	HIS	-	expression tag	UNP B6YWC3
A	437	HIS	-	expression tag	UNP B6YWC3
A	438	HIS	-	expression tag	UNP B6YWC3
B	-1	MET	-	initiating methionine	UNP B6YWC3
B	0	GLY	-	expression tag	UNP B6YWC3
B	433	HIS	-	expression tag	UNP B6YWC3
B	434	HIS	-	expression tag	UNP B6YWC3
B	435	HIS	-	expression tag	UNP B6YWC3
B	436	HIS	-	expression tag	UNP B6YWC3
B	437	HIS	-	expression tag	UNP B6YWC3
B	438	HIS	-	expression tag	UNP B6YWC3
C	-1	MET	-	initiating methionine	UNP B6YWC3
C	0	GLY	-	expression tag	UNP B6YWC3
C	433	HIS	-	expression tag	UNP B6YWC3
C	434	HIS	-	expression tag	UNP B6YWC3
C	435	HIS	-	expression tag	UNP B6YWC3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	436	HIS	-	expression tag	UNP B6YWC3
C	437	HIS	-	expression tag	UNP B6YWC3
C	438	HIS	-	expression tag	UNP B6YWC3
D	-1	MET	-	initiating methionine	UNP B6YWC3
D	0	GLY	-	expression tag	UNP B6YWC3
D	433	HIS	-	expression tag	UNP B6YWC3
D	434	HIS	-	expression tag	UNP B6YWC3
D	435	HIS	-	expression tag	UNP B6YWC3
D	436	HIS	-	expression tag	UNP B6YWC3
D	437	HIS	-	expression tag	UNP B6YWC3
D	438	HIS	-	expression tag	UNP B6YWC3

- Molecule 2 is a RNA chain called RNA (5'-R(*AP*AP*AP*(A23))-3').

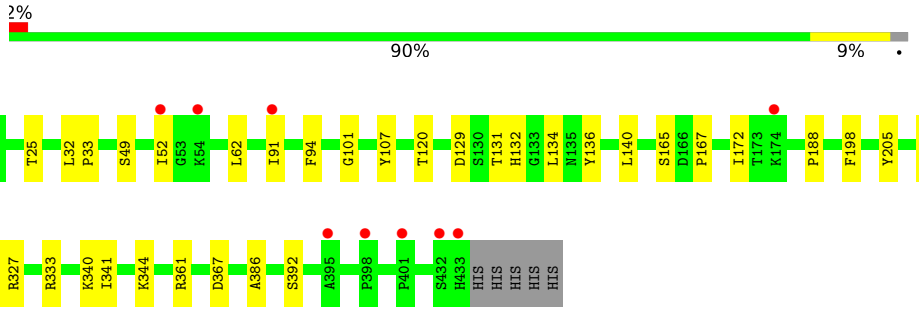
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	4	88	40	20	24	4	0	0	0
2	F	3	48	20	10	15	3	0	0	1
2	G	3	48	20	10	15	3	0	0	1
2	H	4	88	40	20	24	4	0	0	0

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.

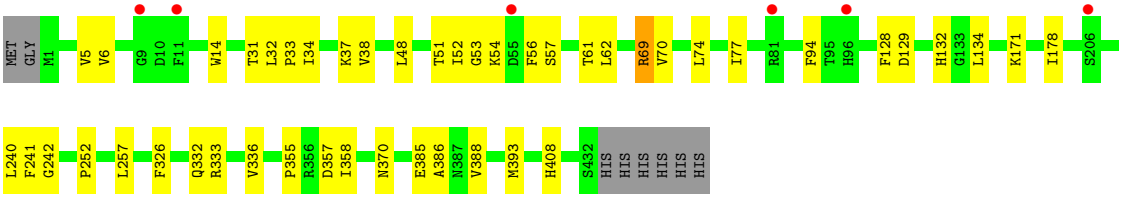
• Molecule 1: Uncharacterized protein

Chain A:



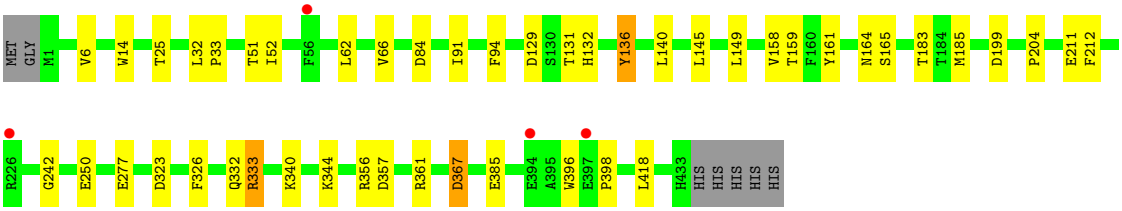
• Molecule 1: Uncharacterized protein

Chain B:



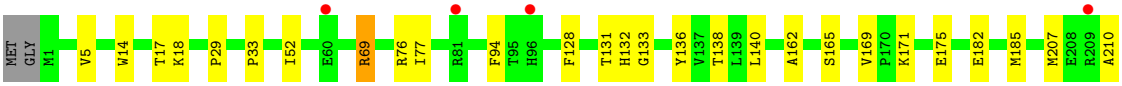
• Molecule 1: Uncharacterized protein

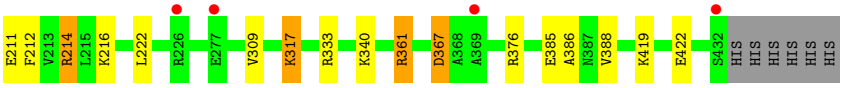
Chain C:



• Molecule 1: Uncharacterized protein

Chain D:





- Molecule 2: RNA (5'-R(*AP*AP*AP*(A23))-3')

Chain E:

- Molecule 2: RNA (5'-R(*AP*AP*AP*(A23))-3')

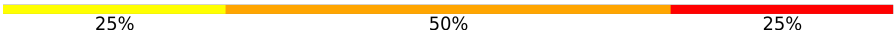
Chain F:

- Molecule 2: RNA (5'-R(*AP*AP*AP*(A23))-3')

Chain G:

- Molecule 2: RNA (5'-R(*AP*AP*AP*(A23))-3')

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.41Å 111.46Å 113.14Å 90.00° 110.01° 90.00°	Depositor
Resolution (Å)	49.41 – 2.80 49.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.41-2.80) 98.7 (49.36-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.214 , 0.257 0.215 , 0.256	Depositor DCC
R_{free} test set	5441 reflections (9.85%)	wwPDB-VP
Wilson B-factor (Å^2)	73.1	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14052	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: A23

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	0.65	0/3526	0.73	0/4772
1	B	0.64	0/3515	0.73	0/4757
1	C	0.65	0/3526	0.73	0/4772
1	D	0.65	0/3515	0.74	0/4757
2	E	0.74	0/71	0.78	0/109
2	F	0.51	0/25	0.90	0/38
2	G	0.15	0/25	0.60	0/38
2	H	0.52	0/71	0.61	0/109
All	All	0.65	0/14274	0.73	0/19352

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3450	0	3499	28	0
1	B	3440	0	3492	42	0
1	C	3450	0	3499	46	0
1	D	3440	0	3492	42	0
2	E	88	0	44	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	48	0	21	8	0
2	G	48	0	21	15	0
2	H	88	0	44	17	0
All	All	14052	0	14112	164	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 164 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:C:51:THR:HG21	1:C:94:PHE:CE1	1.63	1.33
1:C:51:THR:HG21	1:C:94:PHE:CZ	1.73	1.22
1:C:51:THR:CG2	1:C:94:PHE:CE1	2.21	1.21
1:C:340:LYS:NZ	2:G:4:A23:H4'	1.61	1.14
1:C:94:PHE:CD2	2:H:4:A23:N6	2.26	1.04

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	431/440 (98%)	409 (95%)	22 (5%)	0	100	100
1	B	430/440 (98%)	411 (96%)	19 (4%)	0	100	100
1	C	431/440 (98%)	417 (97%)	14 (3%)	0	100	100
1	D	430/440 (98%)	412 (96%)	18 (4%)	0	100	100
All	All	1722/1760 (98%)	1649 (96%)	73 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	372/378 (98%)	366 (98%)	6 (2%)	62	88
1	B	371/378 (98%)	364 (98%)	7 (2%)	57	85
1	C	372/378 (98%)	358 (96%)	14 (4%)	33	67
1	D	371/378 (98%)	362 (98%)	9 (2%)	49	81
All	All	1486/1512 (98%)	1450 (98%)	36 (2%)	49	81

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	76	ARG
1	D	367	ASP
1	D	169	VAL
1	D	214	ARG
1	B	370	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	164	ASN
1	C	179	ASN
1	D	370	ASN
1	B	132	HIS
1	A	370	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	3/4 (75%)	3 (100%)	1 (33%)
2	F	1/4 (25%)	1 (100%)	0
2	G	1/4 (25%)	1 (100%)	0
2	H	3/4 (75%)	3 (100%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	8/16 (50%)	8 (100%)	1 (12%)

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	2	A
2	E	3	A
2	E	4	A23
2	F	4	A23
2	G	4	A23

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	E	2	A

5.4 Non-standard residues in protein, DNA, RNA chains (i)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
2	A23	E	4	2	19,28,29	1.08	1 (5%)	19,43,46	1.74	5 (26%)
2	A23	G	4	2	19,28,29	1.07	1 (5%)	19,43,46	1.73	5 (26%)
2	A23	F	4	2	19,28,29	1.08	1 (5%)	19,43,46	1.72	5 (26%)
2	A23	H	4	2	19,28,29	1.08	1 (5%)	19,43,46	1.74	5 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A23	E	4	2	-	1/3/35/36	0/4/4/4
2	A23	G	4	2	-	2/3/35/36	0/4/4/4
2	A23	F	4	2	-	1/3/35/36	0/4/4/4
2	A23	H	4	2	-	1/3/35/36	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	4	A23	C5-C4	2.51	1.47	1.40
2	E	4	A23	C5-C4	2.50	1.47	1.40
2	F	4	A23	C5-C4	2.50	1.47	1.40
2	G	4	A23	C5-C4	2.47	1.47	1.40

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	4	A23	O2C-PC-O1C	3.53	121.28	109.89
2	F	4	A23	O2C-PC-O1C	3.52	121.27	109.89
2	E	4	A23	O2C-PC-O1C	3.52	121.24	109.89
2	G	4	A23	O2C-PC-O1C	3.51	121.24	109.89
2	E	4	A23	N3-C2-N1	-3.18	123.70	128.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	4	A23	O4'-C4'-C5'-O5'
2	G	4	A23	C3'-C4'-C5'-O5'
2	G	4	A23	O4'-C4'-C5'-O5'
2	H	4	A23	C4'-C5'-O5'-P
2	E	4	A23	C4'-C5'-O5'-P

There are no ring outliers.

4 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	4	A23	7	0
2	G	4	A23	14	0
2	F	4	A23	6	0
2	H	4	A23	11	0

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 (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	433/440 (98%)	0.22	11 (2%)	57	47	57, 78, 114, 144	0
1	B	432/440 (98%)	0.23	6 (1%)	75	70	55, 85, 125, 140	0
1	C	433/440 (98%)	0.19	4 (0%)	84	80	59, 84, 118, 140	0
1	D	432/440 (98%)	0.13	8 (1%)	66	59	59, 79, 117, 139	0
2	E	3/4 (75%)	0.51	0	100	100	113, 113, 140, 140	0
2	F	2/4 (50%)	0.15	0	100	100	122, 122, 122, 140	0
2	G	2/4 (50%)	0.63	0	100	100	136, 136, 136, 155	0
2	H	3/4 (75%)	1.00	0	100	100	120, 120, 126, 139	0
All	All	1740/1776 (97%)	0.20	29 (1%)	70	63	55, 81, 121, 155	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	ARG	5.4
1	A	432	SER	5.0
1	A	433	HIS	3.5
1	B	55	ASP	2.9
1	D	209	ARG	2.7

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95th 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
2	A23	E	4	25/26	0.69	0.31	127,150,154,155	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A23	F	4	25/26	0.76	0.28	116,134,147,150	0
2	A23	G	4	25/26	0.78	0.22	116,141,150,153	0
2	A23	H	4	25/26	0.81	0.29	123,136,148,149	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.