



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:24 AM UTC

PDB ID : 5DCX / pdb\_00005dcx  
Title : Structural studies of AAV2 Rep68 reveal a partially structured linker and compact domain conformation  
Authors : Musayev, F.N.; Zarate-Perez, F.  
Deposited on : 2015-08-24  
Resolution : 2.60 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

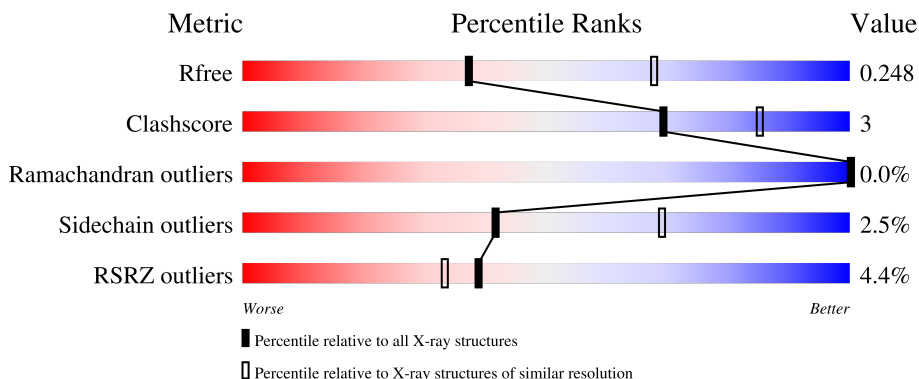
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	227	 4% 82% 9% 8%
1	B	227	 2% 79% 10% 10%
1	C	227	 2% 80% 8% 11%
1	D	227	 2% 79% 9% 11%
1	E	227	 3% 78% 7% 14%

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Mol	Chain	Length	Quality of chain
1	F	227	<p>4% 75% 7% 17%</p>
1	G	227	<p>4% 79% 10% 11%</p>
1	H	227	<p>4% 81% 7% 11%</p>
1	I	227	<p>% 73% 9% 17%</p>
1	J	227	<p>5% 69% 13% 19%</p>
1	K	227	<p>15% 71% 11% 17%</p>

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	MG	A	301	-	-	-	X
2	MG	B	301	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17626 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 Protein Rep68.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	209	Total 1698	C 1091	N 288	O 314	S 5	0	0	0
1	B	205	Total 1675	C 1076	N 284	O 310	S 5	0	0	0
1	C	202	Total 1622	C 1046	N 272	O 298	S 6	0	0	0
1	D	202	Total 1643	C 1057	N 276	O 305	S 5	0	0	0
1	E	195	Total 1594	C 1030	N 267	O 291	S 6	0	0	0
1	F	188	Total 1524	C 988	N 252	O 278	S 6	0	0	0
1	G	203	Total 1620	C 1044	N 276	O 295	S 5	0	0	0
1	H	202	Total 1609	C 1036	N 268	O 300	S 5	0	0	0
1	I	189	Total 1541	C 998	N 255	O 282	S 6	0	0	0
1	J	185	Total 1478	C 957	N 249	O 268	S 4	0	0	0
1	K	189	Total 1438	C 939	N 237	O 256	S 6	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P03132
A	-1	SER	-	expression tag	UNP P03132
A	0	HIS	-	expression tag	UNP P03132
A	151	SER	CYS	engineered mutation	UNP P03132
B	-2	GLY	-	expression tag	UNP P03132
B	-1	SER	-	expression tag	UNP P03132
B	0	HIS	-	expression tag	UNP P03132

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Chain	Residue	Modelled	Actual	Comment	Reference
B	151	SER	CYS	engineered mutation	UNP P03132
C	-2	GLY	-	expression tag	UNP P03132
C	-1	SER	-	expression tag	UNP P03132
C	0	HIS	-	expression tag	UNP P03132
C	151	SER	CYS	engineered mutation	UNP P03132
D	-2	GLY	-	expression tag	UNP P03132
D	-1	SER	-	expression tag	UNP P03132
D	0	HIS	-	expression tag	UNP P03132
D	151	SER	CYS	engineered mutation	UNP P03132
E	-2	GLY	-	expression tag	UNP P03132
E	-1	SER	-	expression tag	UNP P03132
E	0	HIS	-	expression tag	UNP P03132
E	151	SER	CYS	engineered mutation	UNP P03132
F	-2	GLY	-	expression tag	UNP P03132
F	-1	SER	-	expression tag	UNP P03132
F	0	HIS	-	expression tag	UNP P03132
F	151	SER	CYS	engineered mutation	UNP P03132
G	-2	GLY	-	expression tag	UNP P03132
G	-1	SER	-	expression tag	UNP P03132
G	0	HIS	-	expression tag	UNP P03132
G	151	SER	CYS	engineered mutation	UNP P03132
H	-2	GLY	-	expression tag	UNP P03132
H	-1	SER	-	expression tag	UNP P03132
H	0	HIS	-	expression tag	UNP P03132
H	151	SER	CYS	engineered mutation	UNP P03132
I	-2	GLY	-	expression tag	UNP P03132
I	-1	SER	-	expression tag	UNP P03132
I	0	HIS	-	expression tag	UNP P03132
I	151	SER	CYS	engineered mutation	UNP P03132
J	-2	GLY	-	expression tag	UNP P03132
J	-1	SER	-	expression tag	UNP P03132
J	0	HIS	-	expression tag	UNP P03132
J	151	SER	CYS	engineered mutation	UNP P03132
K	-2	GLY	-	expression tag	UNP P03132
K	-1	SER	-	expression tag	UNP P03132
K	0	HIS	-	expression tag	UNP P03132
K	151	SER	CYS	engineered mutation	UNP P03132

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	22	Total O 22 22	0	0
3	B	35	Total O 35 35	0	0
3	C	16	Total O 16 16	0	0
3	D	18	Total O 18 18	0	0
3	E	19	Total O 19 19	0	0
3	F	18	Total O 18 18	0	0
3	G	15	Total O 15 15	0	0

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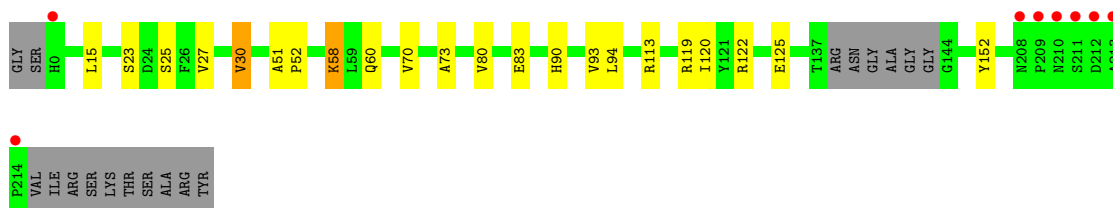
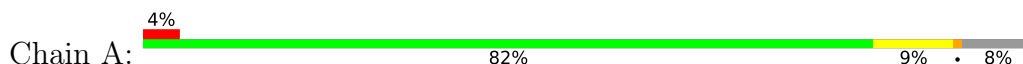
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
3	H	10	Total O 10 10	0	0
3	I	6	Total O 6 6	0	0
3	J	11	Total O 11 11	0	0
3	K	3	Total O 3 3	0	0

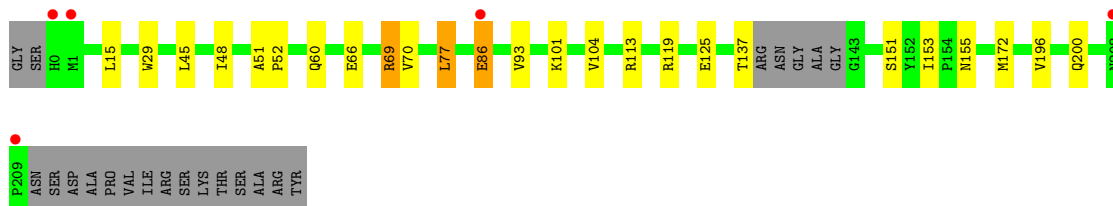
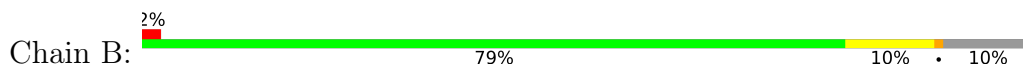
### 3 Residue-property plots [i](#)

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.

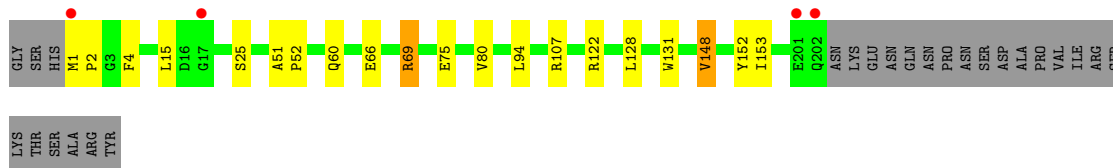
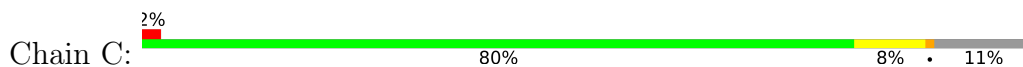
- Molecule 1: Protein Rep68



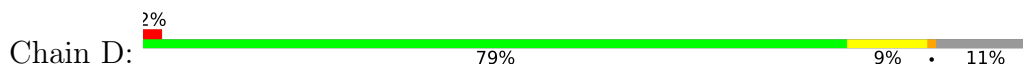
- Molecule 1: Protein Rep68



- Molecule 1: Protein Rep68



- Molecule 1: Protein Rep68





SER GLN THR GLN MET PRO GLN ASN LYS GLN ASN GLN ASN PRO ASN SER ASP ALA PRO VAL ILE ARG SER LYS THR SER ALA ARG TYR

● Molecule 1: Protein Rep68



GLY SER HIS MET PRO G3 K10 L15 G21 V27 P38 P39 D40 E49 Q50 A51 P52 A73 A76 L77 V80 F89 H90 M91 H92 V93 L94 Y95 E96 T97 T98 M103 R107 R119 L128 P129 R138 ASN GLY ALA GLY GLY G144 V147

Y152 I153 P154 L158 E173 Q174 S177 A178 R185 L188 V189 A190 Q191 H192 LEU THR HIS VAL SER GLN THR GLN GLN ASN LYS GLU M91 H92 V93 L94 Y95 E96 T97 T98 M103 R107 R119 L128 P129 R138 ASN GLY ALA GLY GLY G144 V147

● Molecule 1: Protein Rep68



GLY SER HIS M1 P2 L15 D16 G17 H18 W35 P39 D40 S41 D42 M43 D44 L45 M46 L47 I48 D62 T65 Q81 F82 E83 L94 I117 T124 E125 P126 T127 L128 W131 T137 ARG ASN GLY ALA GLY GLY G144 N145 K146 D149 Y152 I153 P154

W55 Y156 L157 P159 T161 Q162 E164 Q174 S177 A178 C179 L180 M181 L182 T183 E184 R185 L188 V189 A190 Q191 H192 L193 T194 H195 VAL SER GLN THR GLN ASN LYS GLU M91 H92 V93 L94 Y95 E96 T97 T98 M103 R107 R119 L128 P129 R138 ASN GLY ALA GLY GLY G144 N145 K146 D149 Y152 I153 P154

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.64Å 178.71Å 130.36Å 90.00° 91.66° 90.00°	Depositor
Resolution (Å)	29.81 – 2.60 29.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.81-2.60) 98.6 (29.81-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.40 (at 2.61Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.191 , 0.237 0.207 , 0.248	Depositor DCC
$R_{free}$ test set	5239 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtrriage
Anisotropy	0.094	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.009 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17626	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: MG

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	0.29	0/1743	0.73	2/2372 (0.1%)
1	B	0.30	0/1719	0.73	2/2337 (0.1%)
1	C	0.28	0/1665	0.74	2/2266 (0.1%)
1	D	0.30	0/1685	0.72	0/2291
1	E	0.28	0/1635	0.74	0/2222
1	F	0.30	0/1565	0.75	0/2129
1	G	0.32	0/1663	0.75	0/2264
1	H	0.29	0/1651	0.70	0/2253
1	I	0.28	0/1583	0.77	4/2154 (0.2%)
1	J	0.29	0/1518	0.76	1/2069 (0.0%)
1	K	0.32	0/1478	0.86	2/2025 (0.1%)
All	All	0.30	0/17905	0.75	13/24382 (0.1%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	125	GLU	CA-C-N	7.54	127.59	119.90
1	K	125	GLU	C-N-CA	7.54	127.59	119.90
1	I	125	GLU	CA-C-N	5.54	126.77	119.84
1	I	125	GLU	C-N-CA	5.54	126.77	119.84
1	I	153	ILE	CA-C-N	-5.27	114.32	119.64

There are no chirality outliers.

There are no planarity outliers.

## 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	1698	0	1660	13	0
1	B	1675	0	1645	15	0
1	C	1622	0	1594	11	0
1	D	1643	0	1608	10	0
1	E	1594	0	1584	9	0
1	F	1524	0	1499	9	0
1	G	1620	0	1585	11	0
1	H	1609	0	1539	8	0
1	I	1541	0	1514	12	0
1	J	1478	0	1420	15	0
1	K	1438	0	1345	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
3	A	22	0	0	1	0
3	B	35	0	0	1	0
3	C	16	0	0	1	0
3	D	18	0	0	0	0
3	E	19	0	0	0	0
3	F	18	0	0	0	0
3	G	15	0	0	1	0
3	H	10	0	0	0	0
3	I	6	0	0	0	0
3	J	11	0	0	0	0
3	K	3	0	0	0	0
All	All	17626	0	16993	120	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 3.

The worst 5 of 120 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:I:173:GLU:HA	1:I:176:LEU:HG	1.63	0.80
1:A:119:ARG:NH1	1:D:21:GLY:O	2.26	0.68
1:B:66:GLU:OE2	1:B:69:ARG:NH2	2.29	0.66
1:C:66:GLU:OE2	1:C:69:ARG:NH1	2.30	0.64
1:A:25:SER:OG	1:A:122:ARG:NH2	2.31	0.63

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	205/227 (90%)	203 (99%)	2 (1%)	0	100	100
1	B	201/227 (88%)	200 (100%)	1 (0%)	0	100	100
1	C	200/227 (88%)	197 (98%)	3 (2%)	0	100	100
1	D	198/227 (87%)	196 (99%)	2 (1%)	0	100	100
1	E	191/227 (84%)	189 (99%)	2 (1%)	0	100	100
1	F	184/227 (81%)	184 (100%)	0	0	100	100
1	G	201/227 (88%)	198 (98%)	3 (2%)	0	100	100
1	H	198/227 (87%)	196 (99%)	2 (1%)	0	100	100
1	I	185/227 (82%)	182 (98%)	3 (2%)	0	100	100
1	J	181/227 (80%)	175 (97%)	6 (3%)	0	100	100
1	K	185/227 (82%)	179 (97%)	5 (3%)	1 (0%)	24	46
All	All	2129/2497 (85%)	2099 (99%)	29 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	194	THR

### 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	186/203 (92%)	183 (98%)	3 (2%)	55 79
1	B	185/203 (91%)	180 (97%)	5 (3%)	39 67
1	C	176/203 (87%)	173 (98%)	3 (2%)	53 78
1	D	180/203 (89%)	171 (95%)	9 (5%)	22 46
1	E	176/203 (87%)	172 (98%)	4 (2%)	44 71
1	F	166/203 (82%)	163 (98%)	3 (2%)	51 76
1	G	173/203 (85%)	169 (98%)	4 (2%)	44 71
1	H	172/203 (85%)	168 (98%)	4 (2%)	44 71
1	I	169/203 (83%)	164 (97%)	5 (3%)	36 64
1	J	155/203 (76%)	151 (97%)	4 (3%)	40 68
1	K	142/203 (70%)	139 (98%)	3 (2%)	47 73
All	All	1880/2233 (84%)	1833 (98%)	47 (2%)	42 69

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	93	VAL
1	I	40	ASP
1	G	147	VAL
1	H	134	VAL
1	I	120	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	145	ASN

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Mol	Chain	Res	Type
1	K	46	ASN
1	G	191	GLN
1	H	192	HIS
1	G	155	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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	209/227 (92%)	-0.12	8 (3%) 44 38	28, 46, 82, 166	0
1	B	205/227 (90%)	-0.21	5 (2%) 59 54	27, 43, 70, 112	0
1	C	202/227 (88%)	-0.25	4 (1%) 65 60	28, 45, 76, 118	0
1	D	202/227 (88%)	-0.28	5 (2%) 58 52	29, 43, 78, 114	0
1	E	195/227 (85%)	-0.15	6 (3%) 51 45	32, 48, 93, 176	0
1	F	188/227 (82%)	-0.13	3 (1%) 70 66	28, 49, 82, 96	0
1	G	203/227 (89%)	0.06	8 (3%) 43 38	36, 57, 90, 125	0
1	H	202/227 (88%)	0.47	8 (3%) 42 37	49, 73, 102, 123	0
1	I	189/227 (83%)	0.14	3 (1%) 70 66	42, 67, 97, 133	0
1	J	185/227 (81%)	0.37	11 (5%) 28 23	33, 69, 111, 138	0
1	K	189/227 (83%)	0.98	34 (17%) 3 3	41, 82, 138, 188	0
All	All	2169/2497 (86%)	0.07	95 (4%) 39 33	27, 55, 104, 188	0

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	213	ALA	6.8
1	A	212	ASP	5.9
1	A	211	SER	5.7
1	J	177	SER	4.8
1	K	192	HIS	4.6

### 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 oligosaccharides 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	MG	B	301	1/1	0.17	0.66	443,443,443,443	0
2	MG	A	301	1/1	0.62	0.53	95,95,95,95	0
2	MG	H	301	1/1	0.92	0.17	46,46,46,46	0
2	MG	D	301	1/1	0.93	0.21	32,32,32,32	0
2	MG	I	301	1/1	0.93	0.18	57,57,57,57	0
2	MG	F	301	1/1	0.94	0.16	39,39,39,39	0
2	MG	G	301	1/1	0.95	0.15	36,36,36,36	0
2	MG	K	301	1/1	0.95	0.12	63,63,63,63	0
2	MG	J	301	1/1	0.96	0.13	48,48,48,48	0
2	MG	C	301	1/1	0.97	0.12	34,34,34,34	0
2	MG	E	301	1/1	0.98	0.10	36,36,36,36	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.