



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 21, 2023 – 12:34 AM EDT

PDB ID : 5KO2  
Title : Mouse pgp 34 linker deleted mutant Hg derivative  
Authors : Xia, D.; Esser, L.; Zhou, F.  
Deposited on : 2016-06-29  
Resolution : 3.30 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](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 : 4.02b-467  
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

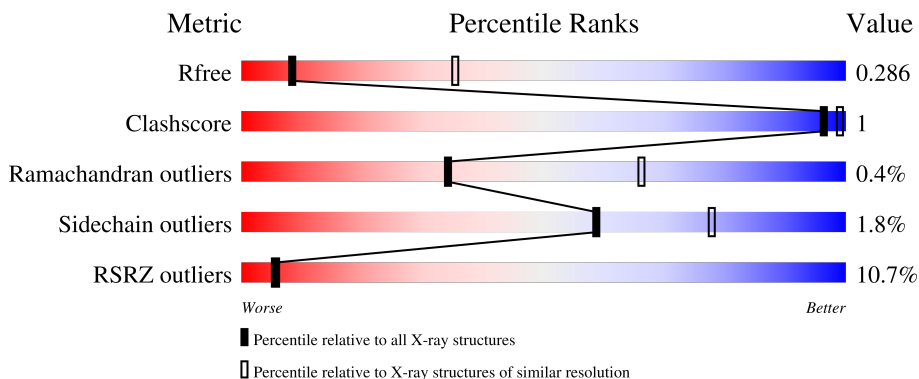
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	1248	 10% 91% 5%
1	B	1248	 11% 90% 5%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 37085 atoms, of which 18697 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 Multidrug resistance protein 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	1185	18539	5907	9350	1559	1685	38	0	0	0
1	B	1184	18532	5905	9347	1558	1684	38	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	GLN	GLU	engineered mutation	UNP P21447
A	?	-	MET	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	LYS	deletion	UNP P21447
A	?	-	ASP	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	GLY	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	LEU	deletion	UNP P21447
A	?	-	ILE	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	THR	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	LYS	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	ILE	deletion	UNP P21447
A	?	-	CYS	deletion	UNP P21447
A	?	-	GLY	deletion	UNP P21447
A	?	-	PRO	deletion	UNP P21447
A	?	-	HIS	deletion	UNP P21447

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P21447
A	?	-	GLN	deletion	UNP P21447
A	?	-	ASP	deletion	UNP P21447
A	?	-	ARG	deletion	UNP P21447
A	?	-	LYS	deletion	UNP P21447
A	?	-	LEU	deletion	UNP P21447
A	?	-	SER	deletion	UNP P21447
A	?	-	THR	deletion	UNP P21447
A	?	-	LYS	deletion	UNP P21447
A	?	-	GLU	deletion	UNP P21447
A	1197	GLN	GLU	engineered mutation	UNP P21447
A	1277	HIS	-	expression tag	UNP P21447
A	1278	HIS	-	expression tag	UNP P21447
A	1279	HIS	-	expression tag	UNP P21447
A	1280	HIS	-	expression tag	UNP P21447
A	1281	HIS	-	expression tag	UNP P21447
A	1282	HIS	-	expression tag	UNP P21447
B	552	GLN	GLU	engineered mutation	UNP P21447
B	?	-	MET	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	LYS	deletion	UNP P21447
B	?	-	ASP	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	GLY	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	LEU	deletion	UNP P21447
B	?	-	ILE	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	THR	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	LYS	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	ILE	deletion	UNP P21447
B	?	-	CYS	deletion	UNP P21447
B	?	-	GLY	deletion	UNP P21447
B	?	-	PRO	deletion	UNP P21447
B	?	-	HIS	deletion	UNP P21447

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	deletion	UNP P21447
B	?	-	GLN	deletion	UNP P21447
B	?	-	ASP	deletion	UNP P21447
B	?	-	ARG	deletion	UNP P21447
B	?	-	LYS	deletion	UNP P21447
B	?	-	LEU	deletion	UNP P21447
B	?	-	SER	deletion	UNP P21447
B	?	-	THR	deletion	UNP P21447
B	?	-	LYS	deletion	UNP P21447
B	?	-	GLU	deletion	UNP P21447
B	1197	GLN	GLU	engineered mutation	UNP P21447
B	1277	HIS	-	expression tag	UNP P21447
B	1278	HIS	-	expression tag	UNP P21447
B	1279	HIS	-	expression tag	UNP P21447
B	1280	HIS	-	expression tag	UNP P21447
B	1281	HIS	-	expression tag	UNP P21447
B	1282	HIS	-	expression tag	UNP P21447

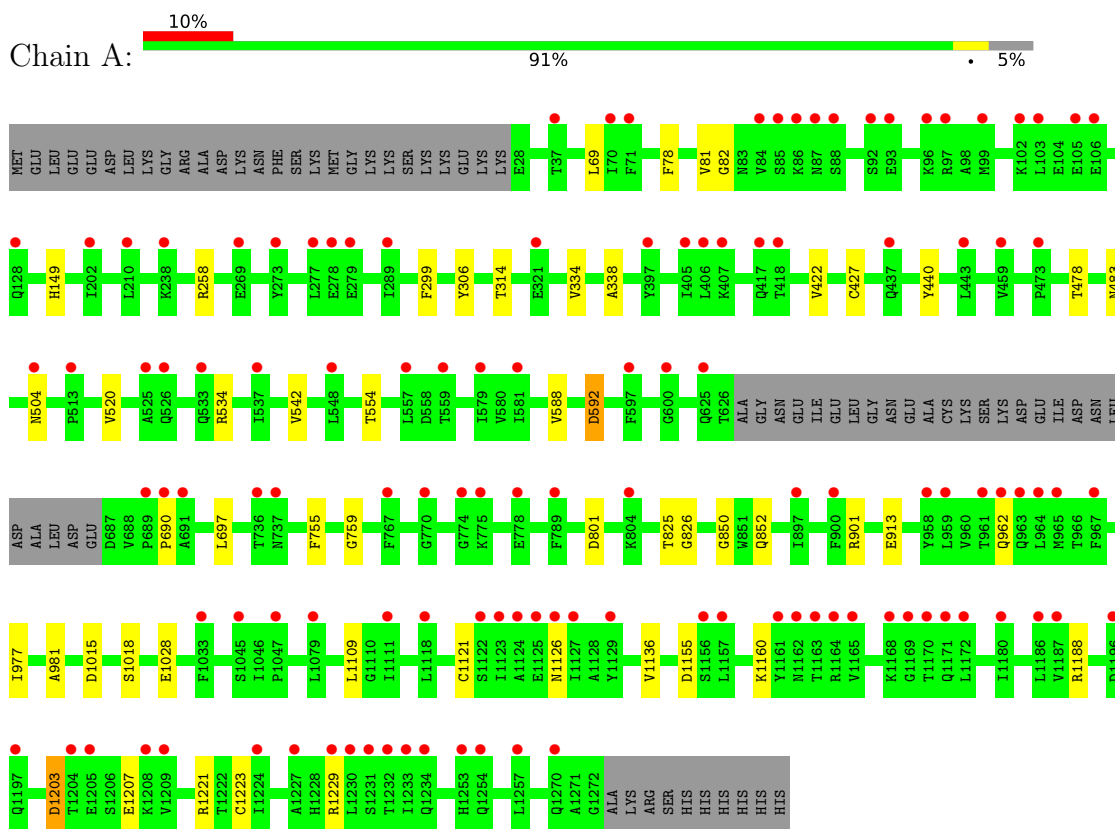
- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	7	Total Hg 7 7	0	0
2	B	7	Total Hg 7 7	0	0

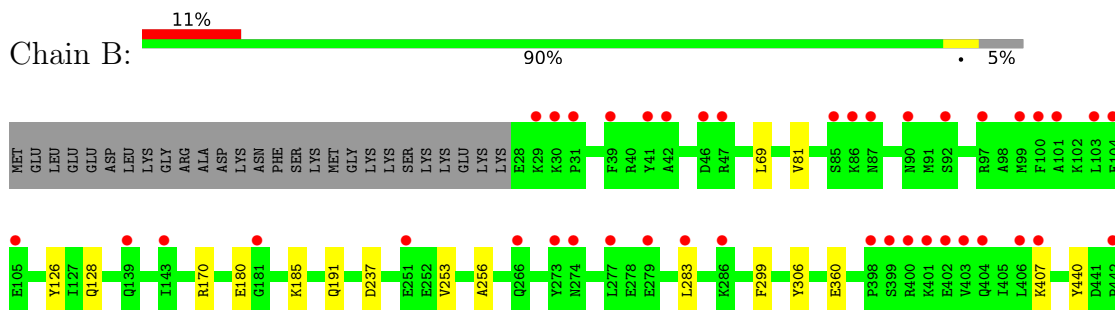
### 3 Residue-property plots

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: Multidrug resistance protein 1A



- Molecule 1: Multidrug resistance protein 1A





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.19Å 114.74Å 375.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.54 – 3.30 49.11 – 3.29	Depositor EDS
% Data completeness (in resolution range)	92.2 (33.54-3.30) 90.5 (49.11-3.29)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 3.33Å)	Xtrriage
Refinement program	PHENIX dev_2443	Depositor
R, $R_{free}$	0.243 , 0.285 0.248 , 0.286	Depositor DCC
$R_{free}$ test set	1966 reflections (3.28%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	108.7	Xtrriage
Anisotropy	0.179	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	37085	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	145.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: HG

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	0/9358	0.50	0/12650
1	B	0.29	0/9354	0.50	0/12645
All	All	0.29	0/18712	0.50	0/25295

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

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	9189	9350	9367	16	0
1	B	9185	9347	9364	21	0
2	A	7	0	0	0	0
2	B	7	0	0	0	0
All	All	18388	18697	18731	37	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 1.

All (37) 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:1134:ARG:NH1	1:B:1140:GLU:OE2	2.26	0.68
1:B:1189:GLN:OE1	1:B:1221:ARG:NH2	2.29	0.65
1:B:440:TYR:OH	1:B:901:ARG:NH2	2.30	0.65
1:A:440:TYR:OH	1:A:901:ARG:NH2	2.31	0.63
1:A:1207:GLU:OE2	1:A:1229:ARG:NH1	2.33	0.61
1:A:852:GLN:N	1:A:852:GLN:OE1	2.34	0.61
1:A:504:ASN:O	1:A:534:ARG:NH2	2.35	0.59
1:B:852:GLN:N	1:B:852:GLN:OE1	2.36	0.57
1:B:942:GLN:N	1:B:942:GLN:OE1	2.37	0.57
1:B:1109:LEU:O	1:B:1188:ARG:NH1	2.36	0.57
1:B:562:GLU:OE1	1:B:584:ARG:NH1	2.38	0.57
1:B:180:GLU:OE2	1:B:185:LYS:NZ	2.34	0.56
1:A:1015:ASP:OD1	1:A:1018:SER:N	2.42	0.53
1:A:1221:ARG:O	1:A:1223:CYS:SG	2.67	0.52
1:A:258:ARG:NH1	1:A:801:ASP:OD1	2.45	0.50
1:B:977:ILE:O	1:B:981:ALA:N	2.38	0.48
1:B:1221:ARG:O	1:B:1223:CYS:SG	2.71	0.48
1:A:977:ILE:O	1:A:981:ALA:N	2.42	0.48
1:A:1109:LEU:O	1:A:1188:ARG:NH1	2.47	0.47
1:B:253:VAL:O	1:B:256:ALA:N	2.47	0.47
1:B:1015:ASP:OD1	1:B:1018:SER:N	2.48	0.47
1:B:1132:ASN:O	1:B:1133:SER:OG	2.28	0.46
1:B:170:ARG:NH1	1:B:360:GLU:OE1	2.48	0.45
1:A:1203:ASP:N	1:A:1203:ASP:OD1	2.47	0.45
1:B:407:LYS:NZ	1:B:599:GLY:O	2.52	0.43
1:A:78:PHE:O	1:A:82:GLY:N	2.50	0.43
1:A:149:HIS:ND1	1:A:913:GLU:OE2	2.30	0.43
1:B:476:PHE:O	1:B:478:THR:N	2.52	0.43
1:B:816:ASN:OD1	1:B:817:ASP:N	2.52	0.43
1:A:334:VAL:O	1:A:338:ALA:N	2.49	0.42
1:B:583:HIS:O	1:B:625:GLN:NE2	2.46	0.41
1:A:755:PHE:O	1:A:759:GLY:N	2.50	0.40
1:B:126:TYR:N	1:B:939:SER:OG	2.54	0.40
1:A:592:ASP:OD1	1:A:592:ASP:N	2.54	0.40
1:A:825:THR:OG1	1:A:826:GLY:N	2.55	0.40
1:B:128:GLN:NE2	1:B:191:GLN:OE1	2.54	0.40
1:B:592:ASP:OD1	1:B:592:ASP:N	2.54	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	1181/1248 (95%)	1139 (96%)	37 (3%)	5 (0%)	34	66
1	B	1180/1248 (95%)	1140 (97%)	35 (3%)	5 (0%)	34	66
All	All	2361/2496 (95%)	2279 (96%)	72 (3%)	10 (0%)	34	66

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1136	VAL
1	B	1160	LYS
1	A	1160	LYS
1	B	1136	VAL
1	A	690	PRO
1	A	1028	GLU
1	B	1028	GLU
1	B	1114	GLN
1	A	850	GLY
1	B	850	GLY

### 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	977/1031 (95%)	957 (98%)	20 (2%)	55	76
1	B	977/1031 (95%)	961 (98%)	16 (2%)	62	79
All	All	1954/2062 (95%)	1918 (98%)	36 (2%)	59	78

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	81	VAL
1	A	299	PHE
1	A	306	TYR
1	A	314	THR
1	A	422	VAL
1	A	427	CYS
1	A	478	THR
1	A	483	ASN
1	A	520	VAL
1	A	542	VAL
1	A	554	THR
1	A	588	VAL
1	A	592	ASP
1	A	697	LEU
1	A	962	GLN
1	A	1121	CYS
1	A	1126	ASN
1	A	1155	ASP
1	A	1203	ASP
1	B	69	LEU
1	B	81	VAL
1	B	237	ASP
1	B	283	LEU
1	B	299	PHE
1	B	306	TYR
1	B	478	THR
1	B	483	ASN
1	B	520	VAL
1	B	542	VAL
1	B	554	THR
1	B	592	ASP
1	B	964	LEU
1	B	1090	VAL
1	B	1096	GLU
1	B	1150	ILE

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

Mol	Chain	Res	Type
1	A	87	ASN

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Mol	Chain	Res	Type
1	B	910	GLN

### 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 14 ligands modelled in this entry, 14 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<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	1185/1248 (94%)	0.70	120 (10%) <b>7</b> <b>6</b>	65, 119, 214, 325	0
1	B	1184/1248 (94%)	0.73	134 (11%) <b>5</b> <b>5</b>	62, 128, 218, 349	0
All	All	2369/2496 (94%)	0.71	254 (10%) <b>6</b> <b>5</b>	62, 123, 218, 349	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1170	THR	12.0
1	A	85	SER	10.1
1	A	690	PRO	9.7
1	A	87	ASN	8.9
1	A	1123	ILE	8.9
1	A	1161	TYR	8.0
1	A	1171	GLN	7.8
1	B	1270	GLN	7.6
1	A	1205	GLU	7.6
1	A	964	LEU	7.4
1	B	1157	LEU	7.2
1	A	88	SER	7.2
1	B	1227	ALA	7.0
1	B	90	ASN	6.7
1	B	1199	THR	6.6
1	B	1156	SER	6.4
1	A	1231	SER	6.2
1	A	1172	LEU	5.7
1	A	1118	LEU	5.7
1	B	1158	PRO	5.6
1	B	1204	THR	5.3
1	B	1159	ASP	5.3
1	A	691	ALA	5.2
1	B	404	GLN	5.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	97	ARG	5.1
1	B	1164	ARG	5.1
1	A	958	TYR	5.0
1	A	1127	ILE	4.8
1	B	1225	VAL	4.8
1	A	1233	ILE	4.8
1	A	737	ASN	4.7
1	B	273	TYR	4.7
1	A	1230	LEU	4.7
1	B	687	ASP	4.6
1	A	1163	THR	4.6
1	B	626	THR	4.6
1	B	279	GLU	4.6
1	B	1226	ILE	4.5
1	B	603	VAL	4.5
1	A	1124	ALA	4.5
1	A	86	LYS	4.4
1	B	286	LYS	4.4
1	B	101	ALA	4.4
1	B	100	PHE	4.2
1	A	775	LYS	4.2
1	B	1160	LYS	4.2
1	B	1271	ALA	4.1
1	B	928	MET	4.1
1	A	689	PRO	4.1
1	A	1234	GLN	4.1
1	A	959	LEU	4.1
1	B	1195	LEU	4.0
1	A	1187	VAL	4.0
1	A	405	ILE	4.0
1	A	1227	ALA	4.0
1	B	786	TYR	3.9
1	B	875	LEU	3.9
1	B	403	VAL	3.9
1	B	1233	ILE	3.9
1	B	1208	LYS	3.9
1	A	269	GLU	3.8
1	B	104	GLU	3.8
1	B	399	SER	3.8
1	A	443	LEU	3.8
1	B	785	ARG	3.8
1	B	87	ASN	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	1122	SER	3.8
1	A	92	SER	3.7
1	A	1162	ASN	3.7
1	B	400	ARG	3.7
1	B	1163	THR	3.7
1	A	1229	ARG	3.6
1	A	770	GLY	3.6
1	B	103	LEU	3.6
1	B	1196	ASP	3.5
1	A	99	MET	3.5
1	B	1231	SER	3.5
1	B	751	PHE	3.5
1	B	407	LYS	3.4
1	B	42	ALA	3.4
1	B	1153	PHE	3.4
1	A	277	LEU	3.4
1	A	1254	GLN	3.4
1	B	744	GLN	3.3
1	B	41	TYR	3.3
1	A	1168	LYS	3.3
1	B	1191	HIS	3.3
1	B	1152	GLN	3.3
1	B	1230	LEU	3.3
1	B	1168	LYS	3.3
1	B	700	ASN	3.3
1	B	1165	VAL	3.3
1	B	878	GLN	3.3
1	A	279	GLU	3.3
1	B	402	GLU	3.3
1	B	1161	TYR	3.3
1	A	1224	ILE	3.2
1	B	99	MET	3.2
1	B	1135	VAL	3.2
1	A	1111	ILE	3.2
1	A	526	GLN	3.1
1	B	991	ALA	3.1
1	B	1154	ILE	3.1
1	A	278	GLU	3.1
1	A	417	GLN	3.1
1	A	581	ILE	3.1
1	A	93	GLU	3.1
1	B	181	GLY	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	398	PRO	3.0
1	B	622	VAL	3.0
1	A	1186	LEU	3.0
1	B	444	ASP	3.0
1	A	1204	THR	3.0
1	A	1125	GLU	3.0
1	B	85	SER	3.0
1	A	962	GLN	3.0
1	B	596	GLY	3.0
1	A	106	GLU	2.9
1	B	604	GLU	2.9
1	A	579	ILE	2.9
1	B	1211	GLN	2.9
1	B	1210	VAL	2.9
1	A	1208	LYS	2.9
1	B	1269	VAL	2.9
1	B	443	LEU	2.9
1	B	30	LYS	2.8
1	B	597	PHE	2.8
1	A	406	LEU	2.8
1	A	1165	VAL	2.8
1	B	522	GLU	2.8
1	A	1079	LEU	2.8
1	B	277	LEU	2.8
1	A	961	THR	2.8
1	B	1224	ILE	2.7
1	A	84	VAL	2.7
1	A	1209	VAL	2.7
1	A	1270	GLN	2.7
1	A	525	ALA	2.7
1	A	897	ILE	2.7
1	B	283	LEU	2.7
1	B	92	SER	2.7
1	A	1232	THR	2.7
1	A	789	PHE	2.7
1	B	814	LEU	2.7
1	A	774	GLY	2.6
1	B	611	LEU	2.6
1	B	736	THR	2.6
1	B	613	ARG	2.6
1	A	273	TYR	2.6
1	A	559	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1203	ASP	2.5
1	A	418	THR	2.5
1	A	1045	SER	2.5
1	A	437	GLN	2.5
1	A	1126	ASN	2.5
1	B	747	ASN	2.5
1	B	401	LYS	2.5
1	A	557	LEU	2.5
1	A	289	ILE	2.5
1	B	934	PHE	2.5
1	B	594	ILE	2.5
1	B	582	ALA	2.5
1	A	1157	LEU	2.5
1	A	1197	GLN	2.5
1	A	965	MET	2.4
1	A	105	GLU	2.4
1	B	1050	GLN	2.4
1	A	600	GLY	2.4
1	B	972	LEU	2.4
1	B	274	ASN	2.4
1	B	1062	LEU	2.4
1	A	537	ILE	2.4
1	B	598	ASP	2.4
1	A	533	GLN	2.4
1	A	103	LEU	2.4
1	B	86	LYS	2.4
1	B	600	GLY	2.4
1	B	1207	GLU	2.4
1	B	585	LEU	2.4
1	B	697	LEU	2.4
1	B	1248	LYS	2.4
1	B	47	ARG	2.4
1	A	504	ASN	2.4
1	A	1169	GLY	2.3
1	A	70	ILE	2.3
1	B	143	ILE	2.3
1	B	857	LEU	2.3
1	B	1123	ILE	2.3
1	A	804	LYS	2.3
1	A	900	PHE	2.3
1	B	1170	THR	2.3
1	A	963	GLN	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	544	ASN	2.3
1	B	949	TYR	2.3
1	B	105	GLU	2.3
1	A	1180	ILE	2.3
1	A	1129	TYR	2.3
1	A	321	GLU	2.3
1	B	1171	GLN	2.3
1	A	1164	ARG	2.3
1	B	523	ARG	2.3
1	A	597	PHE	2.3
1	A	767	PHE	2.3
1	A	967	PHE	2.3
1	B	707	PHE	2.3
1	A	548	LEU	2.2
1	A	37	THR	2.2
1	A	397	TYR	2.2
1	B	266	GLN	2.2
1	B	1079	LEU	2.2
1	B	693	PHE	2.2
1	A	1047	PRO	2.2
1	B	741	PRO	2.2
1	B	1263	TYR	2.2
1	B	97	ARG	2.2
1	B	1229	ARG	2.2
1	B	605	GLN	2.2
1	B	1254	GLN	2.2
1	B	406	LEU	2.2
1	B	1097	ILE	2.2
1	A	128	GLN	2.2
1	A	625	GLN	2.2
1	B	46	ASP	2.2
1	A	210	LEU	2.2
1	A	102	LYS	2.2
1	A	238	LYS	2.2
1	B	29	LYS	2.2
1	A	202	ILE	2.2
1	A	1257	LEU	2.2
1	A	736	THR	2.2
1	B	39	PHE	2.1
1	A	1196	ASP	2.1
1	A	407	LYS	2.1
1	B	251	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1022	LEU	2.1
1	A	1033	PHE	2.1
1	B	526	GLN	2.1
1	A	1156	SER	2.1
1	B	968	GLU	2.1
1	A	96	LYS	2.1
1	B	1193	LEU	2.1
1	A	513	PRO	2.1
1	A	71	PHE	2.1
1	A	459	VAL	2.1
1	A	1253	HIS	2.1
1	A	778	GLU	2.1
1	B	139	GLN	2.0
1	B	1148	ALA	2.0
1	A	473	PRO	2.0
1	B	31	PRO	2.0
1	B	1133	SER	2.0
1	B	442	PRO	2.0
1	B	1232	THR	2.0
1	B	595	ALA	2.0

## 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 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<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	HG	B	1305	1/1	0.61	0.18	347,347,347,347	0
2	HG	B	1307	1/1	0.69	0.28	536,536,536,536	0
2	HG	B	1306	1/1	0.79	0.07	414,414,414,414	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HG	A	1305	1/1	0.79	0.10	303,303,303,303	0
2	HG	A	1307	1/1	0.81	0.24	415,415,415,415	0
2	HG	A	1306	1/1	0.91	0.06	368,368,368,368	0
2	HG	B	1304	1/1	0.93	0.15	385,385,385,385	0
2	HG	A	1304	1/1	0.93	0.13	228,228,228,228	0
2	HG	B	1302	1/1	0.94	0.21	321,321,321,321	0
2	HG	B	1301	1/1	0.96	0.06	182,182,182,182	0
2	HG	A	1301	1/1	0.96	0.09	274,274,274,274	0
2	HG	A	1302	1/1	0.97	0.03	286,286,286,286	0
2	HG	B	1303	1/1	0.98	0.11	142,142,142,142	0
2	HG	A	1303	1/1	0.99	0.07	127,127,127,127	0

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

There are no such residues in this entry.