



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 19, 2017 – 06:20 PM EST

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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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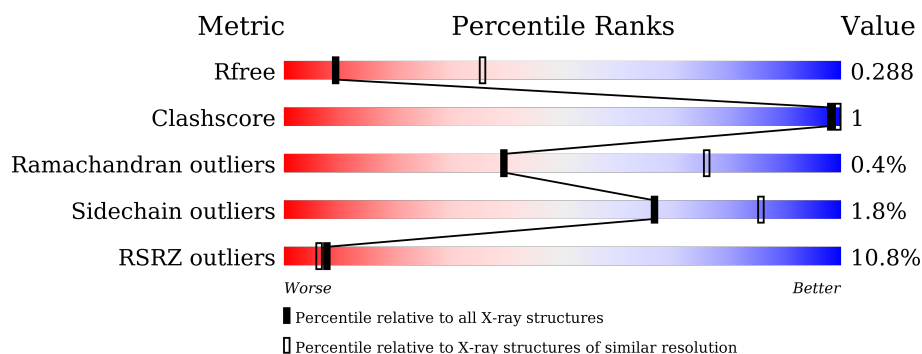
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

**i**

## X-RAY DIFFRACTION

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.



<b>Metric</b>	<b>Whole archive (#Entries)</b>	<b>Similar resolution (#Entries, resolution range(Å))</b>
R <sub>free</sub>	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>10%</div> <div>91%</div> <div>5%</div> </div>
1	B	1248	<div> <div>11%</div> <div>90%</div> <div>5%</div> </div>

## 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
1	A	1185	Total	C	H	N	O	S	0	0	0
			18539	5907	9350	1559	1685	38			
1	B	1184	Total	C	H	N	O	S	0	0	0
			18532	5905	9347	1558	1684	38			

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	?	-	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

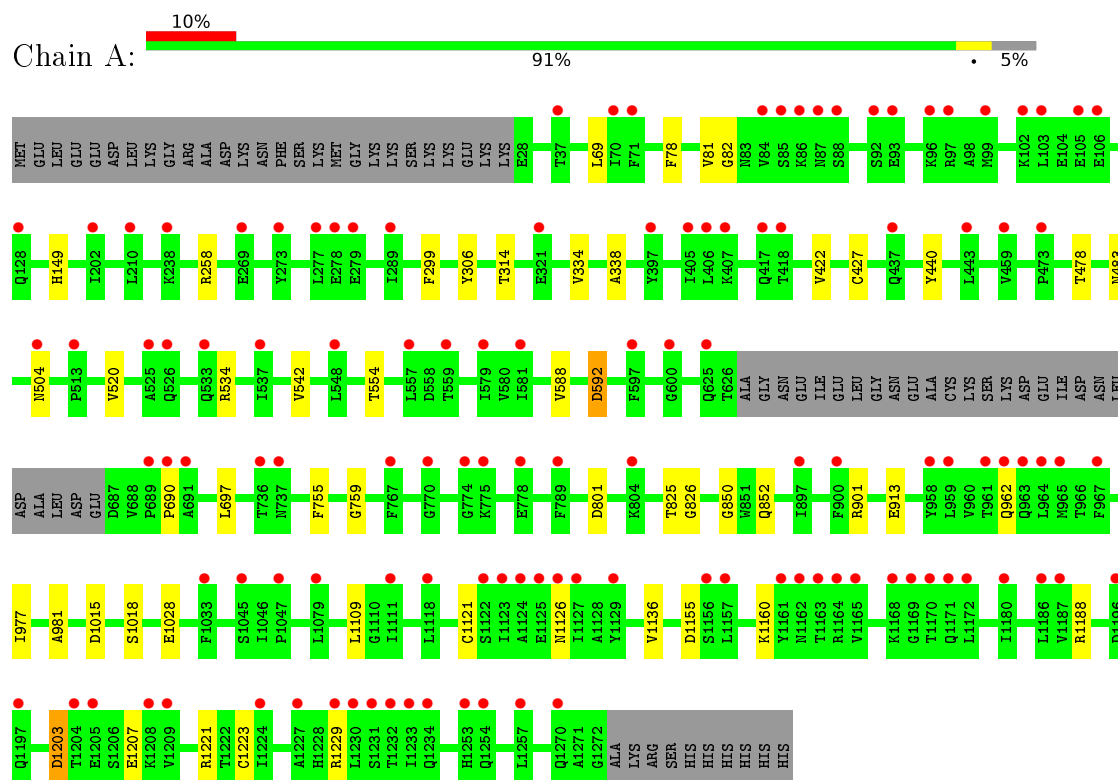
- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

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

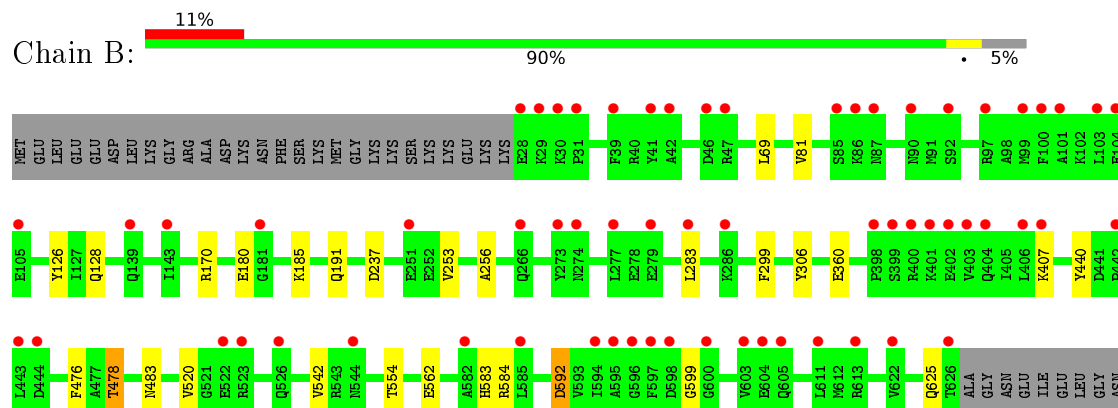
### 3 Residue-property plots

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: 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>	2.37 (at 3.33Å)	Xtriage
Refinement program	PHENIX (dev_2443: ???)	Depositor
R, $R_{free}$	0.243 , 0.285 0.256 , 0.288	Depositor DCC
$R_{free}$ test set	1977 reflections (3.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	105.4	Xtriage
Anisotropy	0.186	Xtriage
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>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	37085	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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:OE1	1:B:852:GLN:N	2.36	0.57
1:B:942:GLN:OE1	1:B:942:GLN:N	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

### 5.3.1 Protein backbone

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%)	39	76
1	B	1180/1248 (95%)	1140 (97%)	35 (3%)	5 (0%)	39	76
All	All	2361/2496 (95%)	2279 (96%)	72 (3%)	10 (0%)	39	76

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

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%)	63	84
1	B	977/1031 (95%)	961 (98%)	16 (2%)	70	87
All	All	1954/2062 (95%)	1918 (98%)	36 (2%)	66	85

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

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	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 carbohydrates 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>9</b> <b>8</b>	65, 119, 214, 325	0
1	B	1184/1248 (94%)	0.73	136 (11%) <b>6</b> <b>5</b>	62, 128, 218, 349	0
All	All	2369/2496 (94%)	0.71	256 (10%) <b>8</b> <b>6</b>	62, 123, 218, 349	0

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1170	THR	12.0
1	A	85	SER	10.2
1	A	690	PRO	9.8
1	A	87	ASN	9.0
1	A	1123	ILE	8.9
1	A	1161	TYR	8.0
1	A	1171	GLN	7.9
1	B	1270	GLN	7.7
1	A	1205	GLU	7.6
1	A	964	LEU	7.4
1	A	88	SER	7.2
1	B	1157	LEU	7.2
1	B	1227	ALA	7.0
1	B	90	ASN	6.7
1	B	1199	THR	6.5
1	B	1156	SER	6.4
1	A	1231	SER	6.2
1	A	1172	LEU	5.8
1	A	1118	LEU	5.7
1	B	1158	PRO	5.6
1	B	1159	ASP	5.3
1	B	1204	THR	5.3
1	A	691	ALA	5.3
1	B	1164	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	97	ARG	5.0
1	B	404	GLN	5.0
1	A	958	TYR	5.0
1	A	1127	ILE	4.9
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	A	1163	THR	4.6
1	B	687	ASP	4.6
1	B	626	THR	4.6
1	B	1226	ILE	4.6
1	B	603	VAL	4.6
1	A	1124	ALA	4.5
1	B	279	GLU	4.5
1	A	86	LYS	4.5
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	4.2
1	A	689	PRO	4.1
1	B	928	MET	4.1
1	B	1195	LEU	4.1
1	A	959	LEU	4.1
1	A	1234	GLN	4.1
1	A	1187	VAL	4.0
1	A	1227	ALA	4.0
1	B	786	TYR	4.0
1	B	875	LEU	4.0
1	A	405	ILE	4.0
1	B	403	VAL	3.9
1	B	399	SER	3.9
1	B	1233	ILE	3.9
1	A	269	GLU	3.9
1	B	1208	LYS	3.9
1	B	104	GLU	3.8
1	B	785	ARG	3.8
1	A	443	LEU	3.8
1	B	87	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1122	SER	3.8
1	B	400	ARG	3.7
1	A	1162	ASN	3.7
1	A	92	SER	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	3.6
1	A	99	MET	3.5
1	B	1231	SER	3.5
1	B	42	ALA	3.5
1	B	751	PHE	3.5
1	B	1153	PHE	3.4
1	A	277	LEU	3.4
1	A	1254	GLN	3.4
1	B	407	LYS	3.4
1	B	41	TYR	3.4
1	B	744	GLN	3.3
1	B	1152	GLN	3.3
1	B	1230	LEU	3.3
1	B	1191	HIS	3.3
1	B	402	GLU	3.3
1	B	1168	LYS	3.3
1	A	1168	LYS	3.3
1	B	878	GLN	3.3
1	A	279	GLU	3.3
1	B	700	ASN	3.3
1	B	1161	TYR	3.2
1	B	1165	VAL	3.2
1	A	1224	ILE	3.2
1	B	1135	VAL	3.2
1	B	99	MET	3.2
1	A	1111	ILE	3.2
1	A	526	GLN	3.2
1	B	991	ALA	3.2
1	B	1154	ILE	3.1
1	A	278	GLU	3.1
1	A	581	ILE	3.1
1	B	398	PRO	3.1
1	A	417	GLN	3.1
1	A	962	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1186	LEU	3.0
1	A	93	GLU	3.0
1	B	85	SER	3.0
1	B	181	GLY	3.0
1	B	604	GLU	3.0
1	B	622	VAL	3.0
1	A	1125	GLU	3.0
1	B	444	ASP	3.0
1	B	596	GLY	3.0
1	A	579	ILE	3.0
1	A	1204	THR	3.0
1	A	106	GLU	2.9
1	B	1211	GLN	2.9
1	B	1269	VAL	2.9
1	B	1210	VAL	2.9
1	A	1208	LYS	2.9
1	A	1165	VAL	2.9
1	B	522	GLU	2.9
1	B	443	LEU	2.8
1	B	597	PHE	2.8
1	A	1079	LEU	2.8
1	B	277	LEU	2.8
1	B	30	LYS	2.8
1	A	406	LEU	2.8
1	A	961	THR	2.8
1	A	84	VAL	2.7
1	B	1224	ILE	2.7
1	A	1232	THR	2.7
1	A	525	ALA	2.7
1	B	92	SER	2.7
1	A	897	ILE	2.7
1	B	814	LEU	2.7
1	A	789	PHE	2.7
1	A	1270	GLN	2.7
1	B	611	LEU	2.7
1	A	1209	VAL	2.7
1	A	774	GLY	2.6
1	B	283	LEU	2.6
1	B	613	ARG	2.6
1	B	736	THR	2.6
1	A	559	THR	2.6
1	A	273	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	401	LYS	2.6
1	A	418	THR	2.6
1	A	437	GLN	2.5
1	A	1126	ASN	2.5
1	A	1045	SER	2.5
1	B	747	ASN	2.5
1	A	557	LEU	2.5
1	A	289	ILE	2.5
1	B	594	ILE	2.5
1	B	1203	ASP	2.5
1	B	934	PHE	2.5
1	B	582	ALA	2.5
1	B	274	ASN	2.5
1	A	1197	GLN	2.4
1	A	105	GLU	2.4
1	A	965	MET	2.4
1	A	1157	LEU	2.4
1	B	972	LEU	2.4
1	A	600	GLY	2.4
1	B	1062	LEU	2.4
1	A	537	ILE	2.4
1	B	86	LYS	2.4
1	B	1248	LYS	2.4
1	B	697	LEU	2.4
1	B	1050	GLN	2.4
1	B	598	ASP	2.4
1	A	533	GLN	2.4
1	A	103	LEU	2.4
1	B	47	ARG	2.4
1	B	1207	GLU	2.4
1	B	585	LEU	2.4
1	B	143	ILE	2.3
1	A	504	ASN	2.3
1	A	1169	GLY	2.3
1	A	70	ILE	2.3
1	B	600	GLY	2.3
1	A	804	LYS	2.3
1	A	900	PHE	2.3
1	B	1170	THR	2.3
1	B	857	LEU	2.3
1	B	949	TYR	2.3
1	A	321	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	523	ARG	2.3
1	B	1171	GLN	2.3
1	B	1123	ILE	2.3
1	A	963	GLN	2.3
1	A	1180	ILE	2.3
1	B	544	ASN	2.3
1	B	105	GLU	2.3
1	A	1164	ARG	2.3
1	A	967	PHE	2.3
1	B	1079	LEU	2.3
1	A	767	PHE	2.3
1	A	1129	TYR	2.3
1	B	605	GLN	2.3
1	A	548	LEU	2.2
1	A	597	PHE	2.2
1	B	693	PHE	2.2
1	B	707	PHE	2.2
1	B	741	PRO	2.2
1	B	266	GLN	2.2
1	B	1229	ARG	2.2
1	A	37	THR	2.2
1	B	1263	TYR	2.2
1	B	97	ARG	2.2
1	B	1097	ILE	2.2
1	A	397	TYR	2.2
1	B	46	ASP	2.2
1	B	29	LYS	2.2
1	A	1047	PRO	2.2
1	B	1254	GLN	2.2
1	A	102	LYS	2.2
1	A	238	LYS	2.2
1	A	210	LEU	2.2
1	A	625	GLN	2.2
1	A	1196	ASP	2.2
1	A	202	ILE	2.2
1	B	406	LEU	2.2
1	A	1033	PHE	2.2
1	B	39	PHE	2.2
1	B	251	GLU	2.2
1	A	736	THR	2.2
1	A	1257	LEU	2.1
1	A	128	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1022	LEU	2.1
1	A	407	LYS	2.1
1	B	968	GLU	2.1
1	A	71	PHE	2.1
1	B	526	GLN	2.1
1	A	778	GLU	2.1
1	B	1193	LEU	2.1
1	A	1253	HIS	2.1
1	A	513	PRO	2.1
1	A	459	VAL	2.1
1	A	96	LYS	2.1
1	B	1148	ALA	2.1
1	A	1156	SER	2.1
1	B	139	GLN	2.1
1	B	595	ALA	2.1
1	A	473	PRO	2.0
1	B	31	PRO	2.0
1	B	442	PRO	2.0
1	B	1133	SER	2.0
1	B	1137	SER	2.0
1	B	28	GLU	2.0
1	B	1232	THR	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 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<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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HG	A	1307	1/1	0.81	0.24	0.63	415,415,415,415	0
2	HG	B	1302	1/1	0.93	0.21	0.03	321,321,321,321	0
2	HG	B	1307	1/1	0.69	0.28	-0.06	536,536,536,536	0
2	HG	B	1305	1/1	0.61	0.18	-0.57	347,347,347,347	0
2	HG	A	1305	1/1	0.78	0.10	-1.09	303,303,303,303	0
2	HG	B	1304	1/1	0.93	0.15	-1.60	385,385,385,385	0
2	HG	A	1303	1/1	0.99	0.07	-1.64	127,127,127,127	0
2	HG	A	1301	1/1	0.96	0.08	-1.70	274,274,274,274	0
2	HG	B	1303	1/1	0.98	0.11	-1.89	142,142,142,142	0
2	HG	A	1304	1/1	0.93	0.13	-2.64	228,228,228,228	0
2	HG	A	1302	1/1	0.97	0.03	-3.47	286,286,286,286	0
2	HG	A	1306	1/1	0.90	0.06	-	368,368,368,368	0
2	HG	B	1306	1/1	0.79	0.07	-	414,414,414,414	0
2	HG	B	1301	1/1	0.96	0.06	-	182,182,182,182	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.