



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:04 am GMT

PDB ID : 4XWS  
Title : OxyR regulatory domain C199D mutant from pseudomonas aeruginosa  
Authors : Jo, I.; Kim, J.S.; Ha, N.C.  
Deposited on : 2015-01-29  
Resolution : 3.01 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

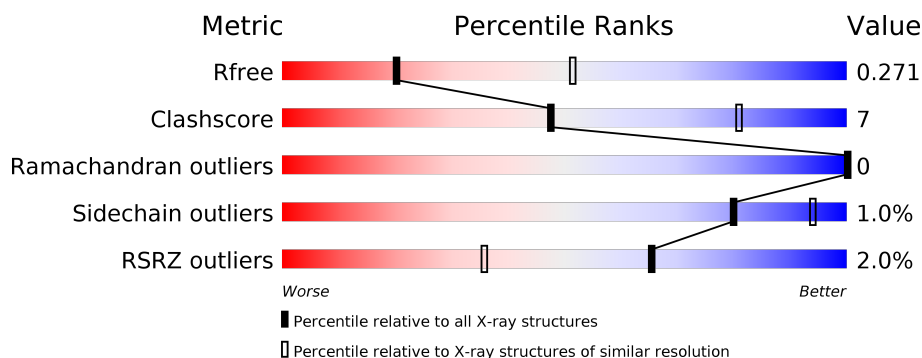
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.01 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))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	227	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>7%</div> </div> </div>
1	B	227	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>19%</div> <div>15%</div> </div> </div>
1	C	227	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>16%</div> <div>•</div> <div>16%</div> </div> </div>
1	D	227	<div> <div></div> <div> <div></div> <div>74%</div> <div>12%</div> <div>15%</div> </div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6176 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 OxyR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1662	1074	285	298	5			
1	B	192	Total	C	N	O	S	0	0	0
			1506	980	254	268	4			
1	C	191	Total	C	N	O	S	0	0	0
			1490	969	251	266	4			
1	D	194	Total	C	N	O	S	0	0	0
			1518	990	255	269	4			

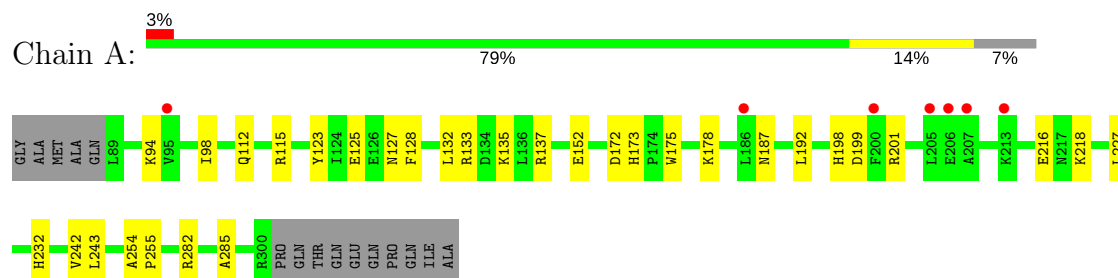
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	GLY	-	expression tag	UNP Q9HTL4
A	85	ALA	-	expression tag	UNP Q9HTL4
A	86	MET	-	expression tag	UNP Q9HTL4
A	87	ALA	-	expression tag	UNP Q9HTL4
A	199	ASP	CYS	engineered mutation	UNP Q9HTL4
B	84	GLY	-	expression tag	UNP Q9HTL4
B	85	ALA	-	expression tag	UNP Q9HTL4
B	86	MET	-	expression tag	UNP Q9HTL4
B	87	ALA	-	expression tag	UNP Q9HTL4
B	199	ASP	CYS	engineered mutation	UNP Q9HTL4
C	84	GLY	-	expression tag	UNP Q9HTL4
C	85	ALA	-	expression tag	UNP Q9HTL4
C	86	MET	-	expression tag	UNP Q9HTL4
C	87	ALA	-	expression tag	UNP Q9HTL4
C	199	ASP	CYS	engineered mutation	UNP Q9HTL4
D	84	GLY	-	expression tag	UNP Q9HTL4
D	85	ALA	-	expression tag	UNP Q9HTL4
D	86	MET	-	expression tag	UNP Q9HTL4
D	87	ALA	-	expression tag	UNP Q9HTL4
D	199	ASP	CYS	engineered mutation	UNP Q9HTL4

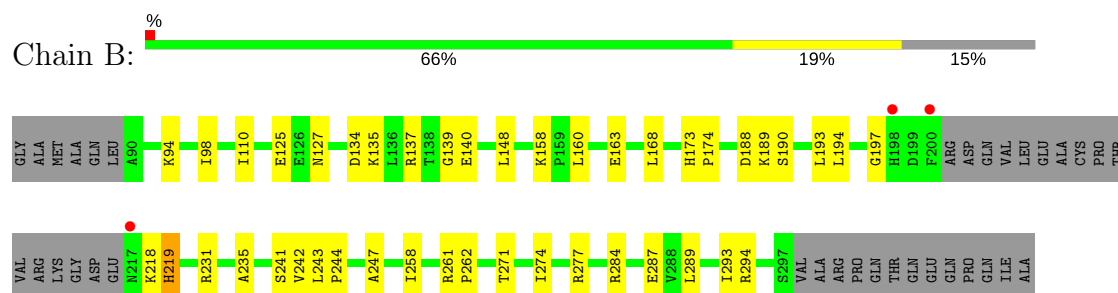
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

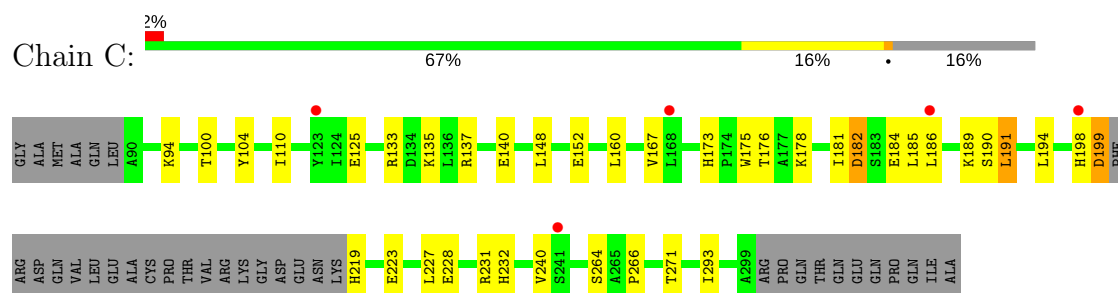
#### • Molecule 1: OxyR



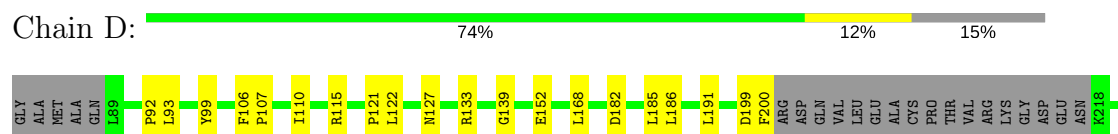
#### • Molecule 1: OxyR

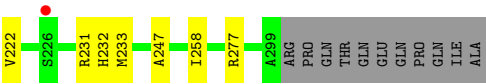


#### • Molecule 1: OxyR



#### • Molecule 1: OxyR





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.94Å 129.94Å 135.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 3.01 43.31 – 3.01	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.99-3.01) 98.1 (43.31-3.01)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.07 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.229 , 0.260 0.234 , 0.271	Depositor DCC
$R_{free}$ test set	1985 reflections (7.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.5	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 5.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.079 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	6176	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	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 23.88 % 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 4.2760e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

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	0.23	0/1708	0.46	0/2333
1	B	0.22	0/1550	0.43	0/2118
1	C	0.25	0/1533	0.52	2/2097 (0.1%)
1	D	0.20	0/1562	0.39	0/2135
All	All	0.23	0/6353	0.45	2/8683 (0.0%)

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	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	199	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	185	LEU	CA-CB-CG	5.32	127.52	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	182	ASP	Peptide

### 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	1662	0	1677	20	0
1	B	1506	0	1515	28	0
1	C	1490	0	1501	27	0
1	D	1518	0	1534	15	0
All	All	6176	0	6227	87	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 7.

All (87) 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:158:LYS:HE2	1:B:294:ARG:HH12	1.33	0.91
1:C:100:THR:HG22	1:C:227:LEU:HD21	1.51	0.91
1:B:193:LEU:HD12	1:B:219:HIS:CD2	2.14	0.82
1:C:125:GLU:OE2	1:C:135:LYS:NZ	2.13	0.81
1:C:194:LEU:H	1:C:198:HIS:HD2	1.28	0.80
1:C:137:ARG:HH12	1:C:152:GLU:HB3	1.47	0.80
1:B:134:ASP:OD1	1:B:137:ARG:NH1	2.15	0.79
1:B:231:ARG:NH2	1:B:247:ALA:O	2.18	0.76
1:C:194:LEU:H	1:C:198:HIS:CD2	2.02	0.76
1:B:173:HIS:HD2	1:B:174:PRO:HD2	1.53	0.74
1:B:158:LYS:HE2	1:B:294:ARG:NH1	2.06	0.71
1:A:187:ASN:ND2	1:A:216:GLU:OE1	2.25	0.70
1:B:284:ARG:NH1	1:B:287:GLU:OE2	2.25	0.69
1:C:133:ARG:HH11	1:C:137:ARG:HH21	1.40	0.69
1:C:137:ARG:NH1	1:C:152:GLU:HB3	2.10	0.65
1:C:194:LEU:HB2	1:C:198:HIS:CD2	2.32	0.65
1:B:193:LEU:HD12	1:B:219:HIS:HD2	1.58	0.65
1:C:181:ILE:O	1:C:264:SER:N	2.30	0.64
1:B:158:LYS:CE	1:B:294:ARG:HH12	2.10	0.63
1:C:182:ASP:OD2	1:C:266:PRO:HD2	1.98	0.63
1:B:139:GLY:HA2	1:B:277:ARG:NH1	2.15	0.62
1:A:137:ARG:NH2	1:A:152:GLU:OE1	2.32	0.62
1:D:182:ASP:HB2	1:D:185:LEU:HD13	1.82	0.60
1:B:125:GLU:OE2	1:B:135:LYS:NZ	2.24	0.60
1:D:168:LEU:HD11	1:D:258:ILE:HD12	1.83	0.60
1:C:133:ARG:NH1	1:C:137:ARG:HH21	2.00	0.59
1:D:186:LEU:HD22	1:D:191:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ALA:HB2	1:B:258:ILE:HD11	1.88	0.56
1:D:92:PRO:HA	1:D:121:PRO:HG2	1.88	0.55
1:D:231:ARG:NH2	1:D:247:ALA:O	2.31	0.54
1:C:160:LEU:HD13	1:C:293:ILE:HG21	1.89	0.54
1:A:216:GLU:HB3	1:A:218:LYS:HE2	1.90	0.52
1:B:163:GLU:OE2	1:B:244:PRO:HB2	2.09	0.52
1:A:218:LYS:N	1:A:218:LYS:HD3	2.25	0.52
1:D:222:VAL:HG11	1:D:233:MET:HE1	1.92	0.51
1:D:133:ARG:NH1	1:D:152:GLU:HG2	2.25	0.51
1:C:175:TRP:CD1	1:C:178:LYS:NZ	2.79	0.51
1:A:175:TRP:HA	1:A:178:LYS:HE2	1.93	0.50
1:A:198:HIS:NE2	1:A:242:VAL:O	2.34	0.50
1:C:110:ILE:HG21	1:D:232:HIS:CG	2.46	0.50
1:A:128:PHE:O	1:A:132:LEU:HB2	2.12	0.49
1:A:282:ARG:HD2	1:A:285:ALA:HB2	1.94	0.49
1:D:93:LEU:HB3	1:D:122:LEU:HD23	1.95	0.49
1:A:172:ASP:OD1	1:A:173:HIS:N	2.45	0.48
1:B:194:LEU:HB2	1:B:197:GLY:HA3	1.94	0.48
1:C:189:LYS:HA	1:C:219:HIS:HA	1.95	0.48
1:D:139:GLY:HA2	1:D:277:ARG:NH1	2.29	0.47
1:B:193:LEU:CD1	1:B:219:HIS:HD2	2.26	0.47
1:A:94:LYS:HA	1:A:123:TYR:HB3	1.96	0.47
1:B:168:LEU:HD13	1:B:243:LEU:HD12	1.97	0.47
1:C:198:HIS:CE1	1:C:227:LEU:HD22	2.51	0.46
1:A:125:GLU:OE2	1:A:135:LYS:NZ	2.30	0.46
1:D:199:ASP:OD1	1:D:200:PHE:N	2.48	0.46
1:A:133:ARG:HD3	1:A:152:GLU:HG3	1.98	0.46
1:C:232:HIS:CG	1:D:110:ILE:HG21	2.50	0.46
1:C:148:LEU:HB2	1:C:271:THR:HB	1.98	0.45
1:B:94:LYS:HD2	1:B:140:GLU:O	2.16	0.45
1:C:104:TYR:OH	1:C:227:LEU:HB2	2.17	0.45
1:C:186:LEU:O	1:C:191:LEU:HD22	2.17	0.45
1:C:133:ARG:HH11	1:C:137:ARG:NH2	2.08	0.45
1:A:133:ARG:NH1	1:A:152:GLU:OE2	2.50	0.44
1:D:99:TYR:CZ	1:D:127:ASN:HA	2.52	0.44
1:B:173:HIS:HD2	1:B:174:PRO:CD	2.26	0.44
1:C:194:LEU:N	1:C:198:HIS:HD2	2.05	0.44
1:B:160:LEU:HD11	1:B:274:ILE:HB	1.99	0.44
1:B:148:LEU:HB2	1:B:271:THR:HB	1.98	0.44
1:A:254:ALA:HA	1:A:255:PRO:HD3	1.93	0.43
1:A:232:HIS:CG	1:B:110:ILE:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:LEU:O	1:B:293:ILE:HG13	2.18	0.43
1:B:98:ILE:HA	1:B:127:ASN:O	2.19	0.43
1:B:261:ARG:HA	1:B:262:PRO:HD3	1.88	0.43
1:B:188:ASP:HB3	1:B:190:SER:H	1.84	0.43
1:C:94:LYS:HD2	1:C:140:GLU:O	2.19	0.42
1:A:227:LEU:HD13	1:A:243:LEU:HD22	2.02	0.42
1:D:115:ARG:HB2	1:D:115:ARG:HE	1.65	0.41
1:A:112:GLN:HG2	1:A:115:ARG:HH22	1.84	0.41
1:C:228:GLU:OE2	1:C:231:ARG:NH2	2.53	0.41
1:C:173:HIS:O	1:C:176:THR:HG22	2.21	0.41
1:C:175:TRP:HZ3	1:C:240:VAL:HG21	1.86	0.41
1:A:216:GLU:HB3	1:A:218:LYS:HG2	2.02	0.41
1:B:218:LYS:HD2	1:B:218:LYS:HA	1.71	0.41
1:C:167:VAL:HG21	1:C:181:ILE:HG21	2.03	0.41
1:D:106:PHE:N	1:D:107:PRO:HD2	2.36	0.41
1:A:98:ILE:HA	1:A:127:ASN:O	2.21	0.40
1:B:241:SER:OG	1:B:242:VAL:N	2.53	0.40
1:B:189:LYS:HD3	1:B:189:LYS:HA	1.94	0.40
1:A:199:ASP:OD2	1:A:201:ARG:HG3	2.22	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	210/227 (92%)	198 (94%)	12 (6%)	0	100	100
1	B	188/227 (83%)	175 (93%)	13 (7%)	0	100	100
1	C	187/227 (82%)	176 (94%)	11 (6%)	0	100	100
1	D	190/227 (84%)	184 (97%)	6 (3%)	0	100	100
All	All	775/908 (85%)	733 (95%)	42 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	182/193 (94%)	181 (100%)	1 (0%)	91	97
1	B	165/193 (86%)	164 (99%)	1 (1%)	89	96
1	C	163/193 (84%)	158 (97%)	5 (3%)	45	80
1	D	166/193 (86%)	166 (100%)	0	100	100
All	All	676/772 (88%)	669 (99%)	7 (1%)	80	94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	LEU
1	B	219	HIS
1	C	184	GLU
1	C	190	SER
1	C	191	LEU
1	C	199	ASP
1	C	223	GLU

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

Mol	Chain	Res	Type
1	B	173	HIS
1	C	198	HIS

### 5.3.3 RNA ⓘ

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](#)

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, 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	212/227 (93%)	0.13	7 (3%)	47	21	36, 61, 105, 138	0
1	B	192/227 (84%)	0.11	3 (1%)	72	44	38, 55, 84, 104	0
1	C	191/227 (84%)	0.09	5 (2%)	56	27	33, 62, 107, 122	0
1	D	194/227 (85%)	-0.07	1 (0%)	90	74	34, 49, 69, 78	0
All	All	789/908 (86%)	0.07	16 (2%)	65	36	33, 56, 99, 138	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	ASN	6.1
1	C	186	LEU	4.0
1	B	200	PHE	3.8
1	A	205	LEU	3.8
1	C	198	HIS	3.4
1	A	207	ALA	3.2
1	B	198	HIS	3.0
1	A	206	GLU	2.9
1	C	168	LEU	2.9
1	C	241	SER	2.6
1	A	95	VAL	2.5
1	A	213	LYS	2.4
1	A	186	LEU	2.4
1	D	226	SER	2.2
1	A	200	PHE	2.2
1	C	123	TYR	2.1

### 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](#)

There are no ligands in this entry.

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

There are no such residues in this entry.