



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:31 PM GMT

PDB ID : 4Y0M
Title : The reduced form of OxyR regulatory domain from *Pseudomonas aeruginosa*
Authors : Jo, I.; Kim, J.S.; Ha, N.C.
Deposited on : 2015-02-06
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

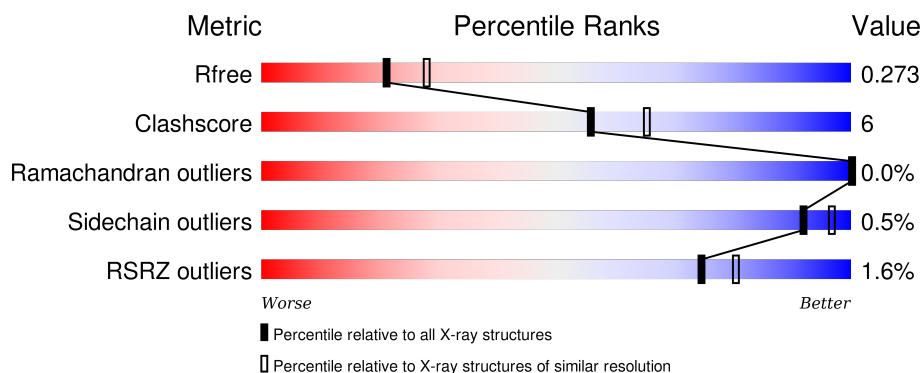
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 ≥ 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></div> <div>76% 13% 11%</div> </div>
1	B	227	<div> <div></div> <div>77% 14% 10%</div> </div>
1	C	227	<div> <div></div> <div>81% 9% 9%</div> </div>
1	D	227	<div> <div></div> <div>77% 12% 11%</div> </div>
1	E	227	<div> <div></div> <div>73% 15% 12%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	227	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>78%</div><div>13%</div><div>9%</div></div></div>
1	G	227	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>78%</div><div>12%</div><div>9%</div></div></div>
1	H	227	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>76%</div><div>12%</div><div>• 11%</div></div></div>
1	I	227	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>80%</div><div>9%</div><div>11%</div></div></div>
1	J	227	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>77%</div><div>15%</div><div>• 8%</div></div></div>
1	K	227	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>78%</div><div>13%</div><div>9%</div></div></div>
1	L	227	<div><div><div></div><div></div><div></div></div><div><div>4%</div><div>74%</div><div>14%</div><div>11%</div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19492 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	203	Total	C	N	O	S	Se	0	0	0
			1590	1032	270	282	3	3			
1	B	205	Total	C	N	O	S	Se	0	0	0
			1603	1040	272	285	3	3			
1	C	206	Total	C	N	O	S	Se	0	1	0
			1618	1049	275	288	3	3			
1	D	203	Total	C	N	O	S	Se	0	0	0
			1588	1031	269	282	3	3			
1	E	200	Total	C	N	O	S	Se	0	0	0
			1568	1019	265	278	3	3			
1	F	207	Total	C	N	O	S	Se	0	0	0
			1621	1051	277	287	3	3			
1	G	206	Total	C	N	O	S	Se	0	0	0
			1609	1044	274	285	3	3			
1	H	202	Total	C	N	O	S	Se	0	0	0
			1582	1028	268	280	3	3			
1	I	202	Total	C	N	O	S	Se	0	0	0
			1579	1025	267	281	3	3			
1	J	209	Total	C	N	O	S	Se	0	0	0
			1632	1059	278	289	3	3			
1	K	206	Total	C	N	O	S	Se	0	0	0
			1613	1047	275	285	3	3			
1	L	201	Total	C	N	O	S	Se	0	0	0
			1573	1022	266	279	3	3			

There are 48 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	MSE	-	expression tag	UNP Q9HTL4
A	87	ALA	-	expression tag	UNP Q9HTL4
B	84	GLY	-	expression tag	UNP Q9HTL4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ALA	-	expression tag	UNP Q9HTL4
B	86	MSE	-	expression tag	UNP Q9HTL4
B	87	ALA	-	expression tag	UNP Q9HTL4
C	84	GLY	-	expression tag	UNP Q9HTL4
C	85	ALA	-	expression tag	UNP Q9HTL4
C	86	MSE	-	expression tag	UNP Q9HTL4
C	87	ALA	-	expression tag	UNP Q9HTL4
D	84	GLY	-	expression tag	UNP Q9HTL4
D	85	ALA	-	expression tag	UNP Q9HTL4
D	86	MSE	-	expression tag	UNP Q9HTL4
D	87	ALA	-	expression tag	UNP Q9HTL4
E	84	GLY	-	expression tag	UNP Q9HTL4
E	85	ALA	-	expression tag	UNP Q9HTL4
E	86	MSE	-	expression tag	UNP Q9HTL4
E	87	ALA	-	expression tag	UNP Q9HTL4
F	84	GLY	-	expression tag	UNP Q9HTL4
F	85	ALA	-	expression tag	UNP Q9HTL4
F	86	MSE	-	expression tag	UNP Q9HTL4
F	87	ALA	-	expression tag	UNP Q9HTL4
G	84	GLY	-	expression tag	UNP Q9HTL4
G	85	ALA	-	expression tag	UNP Q9HTL4
G	86	MSE	-	expression tag	UNP Q9HTL4
G	87	ALA	-	expression tag	UNP Q9HTL4
H	84	GLY	-	expression tag	UNP Q9HTL4
H	85	ALA	-	expression tag	UNP Q9HTL4
H	86	MSE	-	expression tag	UNP Q9HTL4
H	87	ALA	-	expression tag	UNP Q9HTL4
I	84	GLY	-	expression tag	UNP Q9HTL4
I	85	ALA	-	expression tag	UNP Q9HTL4
I	86	MSE	-	expression tag	UNP Q9HTL4
I	87	ALA	-	expression tag	UNP Q9HTL4
J	84	GLY	-	expression tag	UNP Q9HTL4
J	85	ALA	-	expression tag	UNP Q9HTL4
J	86	MSE	-	expression tag	UNP Q9HTL4
J	87	ALA	-	expression tag	UNP Q9HTL4
K	84	GLY	-	expression tag	UNP Q9HTL4
K	85	ALA	-	expression tag	UNP Q9HTL4
K	86	MSE	-	expression tag	UNP Q9HTL4
K	87	ALA	-	expression tag	UNP Q9HTL4
L	84	GLY	-	expression tag	UNP Q9HTL4
L	85	ALA	-	expression tag	UNP Q9HTL4
L	86	MSE	-	expression tag	UNP Q9HTL4

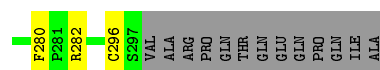
Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	87	ALA	-	expression tag	UNP Q9HTL4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	15	Total O 15 15	0	0
2	B	16	Total O 16 16	0	0
2	C	30	Total O 30 30	0	0
2	D	28	Total O 28 28	0	0
2	E	31	Total O 31 31	0	0
2	F	35	Total O 35 35	0	0
2	G	40	Total O 40 40	0	0
2	H	17	Total O 17 17	0	0
2	I	35	Total O 35 35	0	0
2	J	40	Total O 40 40	0	0
2	K	23	Total O 23 23	0	0
2	L	6	Total O 6 6	0	0



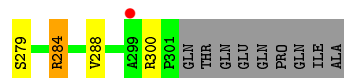
- Molecule 1: OxyR

Chain E: 73% 15% 12%



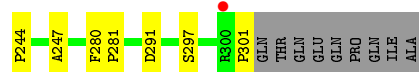
- Molecule 1: OxyR

Chain F: 2% 78% 13% 9%



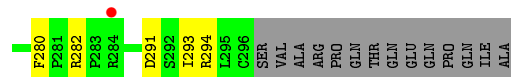
- Molecule 1: OxyR

Chain G: 0% 78% 12% 9%



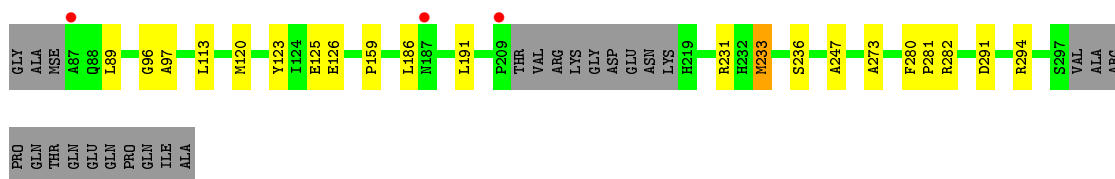
- Molecule 1: OxyR

Chain H: 2% 76% 12% 11%

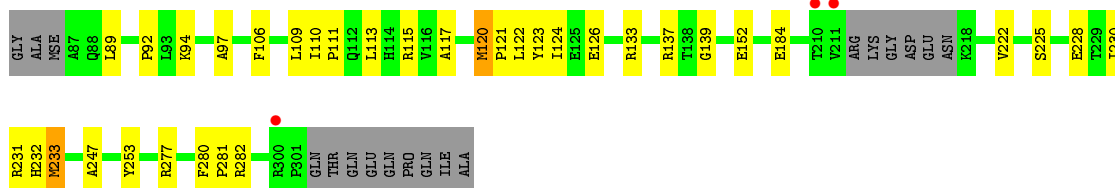
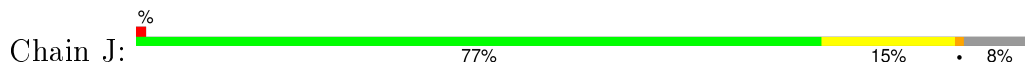


- Molecule 1: OxyR

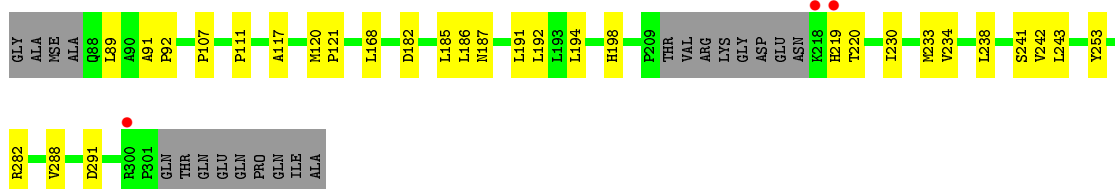
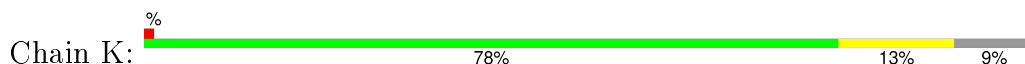
Chain I: 0% 80% 9% 11%



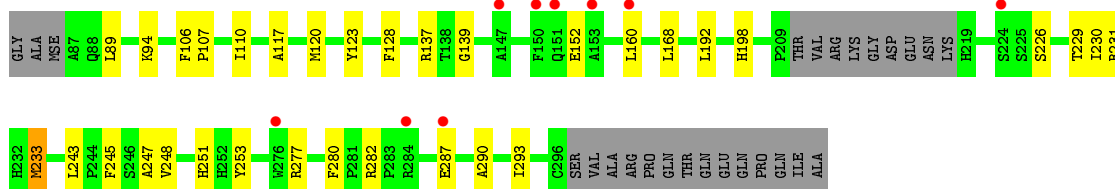
• Molecule 1: OxyR



• Molecule 1: OxyR



• Molecule 1: OxyR



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	151.35Å 151.35Å 218.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.89 – 2.30 44.34 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.89-2.30) 99.4 (44.34-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.217 , 0.271 0.217 , 0.273	Depositor DCC
R_{free} test set	6322 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.7	EDS
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	5 of 126211 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19492	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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 62.68 % 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 1.0861e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.36	0/1632	0.57	2/2225 (0.1%)
1	B	0.36	0/1645	0.54	0/2244
1	C	0.37	0/1661	0.57	2/2266 (0.1%)
1	D	0.40	0/1630	0.59	1/2222 (0.0%)
1	E	0.40	0/1610	0.57	2/2196 (0.1%)
1	F	0.37	0/1664	0.56	0/2269
1	G	0.42	0/1652	0.57	1/2254 (0.0%)
1	H	0.37	0/1624	0.56	2/2214 (0.1%)
1	I	0.40	0/1621	0.58	1/2211 (0.0%)
1	J	0.40	0/1675	0.60	3/2285 (0.1%)
1	K	0.35	0/1656	0.52	0/2258
1	L	0.33	0/1615	0.53	1/2203 (0.0%)
All	All	0.38	0/19685	0.56	15/26847 (0.1%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	233	MSE	CA-CB-CG	8.68	128.05	113.30
1	C	233	MSE	CA-CB-CG	8.06	127.00	113.30
1	A	233	MSE	CA-CB-CG	7.81	126.57	113.30
1	J	233	MSE	CA-CB-CG	7.71	126.40	113.30
1	E	233	MSE	CA-CB-CG	7.47	126.00	113.30

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	1590	0	1603	21	0
1	B	1603	0	1619	23	0
1	C	1618	0	1628	14	0
1	D	1588	0	1602	22	0
1	E	1568	0	1579	22	0
1	F	1621	0	1637	21	0
1	G	1609	0	1623	22	0
1	H	1582	0	1597	19	0
1	I	1579	0	1589	15	0
1	J	1632	0	1652	29	0
1	K	1613	0	1631	19	0
1	L	1573	0	1584	26	0
2	A	15	0	0	0	0
2	B	16	0	0	0	0
2	C	30	0	0	0	0
2	D	28	0	0	0	0
2	E	31	0	0	0	0
2	F	35	0	0	0	0
2	G	40	0	0	0	0
2	H	17	0	0	0	0
2	I	35	0	0	0	0
2	J	40	0	0	0	0
2	K	23	0	0	0	0
2	L	6	0	0	1	0
All	All	19492	0	19344	240	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 240 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:J:117:ALA:HB1	1:J:120:MSE:HE3	1.37	1.07
1:L:117:ALA:HB1	1:L:120:MSE:HE3	1.45	0.98
1:D:117:ALA:HB1	1:D:120:MSE:HE3	1.43	0.97
1:D:89:LEU:HD22	1:D:120:MSE:HE1	1.46	0.94
1:H:231:ARG:NH2	1:H:247:ALA:O	2.09	0.86

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	199/227 (88%)	195 (98%)	4 (2%)	0	100	100
1	B	201/227 (88%)	195 (97%)	6 (3%)	0	100	100
1	C	203/227 (89%)	198 (98%)	4 (2%)	1 (0%)	34	41
1	D	199/227 (88%)	195 (98%)	4 (2%)	0	100	100
1	E	196/227 (86%)	190 (97%)	6 (3%)	0	100	100
1	F	203/227 (89%)	198 (98%)	5 (2%)	0	100	100
1	G	202/227 (89%)	199 (98%)	3 (2%)	0	100	100
1	H	198/227 (87%)	194 (98%)	4 (2%)	0	100	100
1	I	198/227 (87%)	194 (98%)	4 (2%)	0	100	100
1	J	205/227 (90%)	201 (98%)	4 (2%)	0	100	100
1	K	202/227 (89%)	198 (98%)	4 (2%)	0	100	100
1	L	197/227 (87%)	191 (97%)	6 (3%)	0	100	100
All	All	2403/2724 (88%)	2348 (98%)	54 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	299	ALA

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	174/189 (92%)	174 (100%)	0	100	100
1	B	176/189 (93%)	175 (99%)	1 (1%)	90	96
1	C	177/189 (94%)	177 (100%)	0	100	100
1	D	174/189 (92%)	171 (98%)	3 (2%)	68	83
1	E	172/189 (91%)	172 (100%)	0	100	100
1	F	178/189 (94%)	175 (98%)	3 (2%)	68	83
1	G	176/189 (93%)	175 (99%)	1 (1%)	90	96
1	H	173/189 (92%)	172 (99%)	1 (1%)	90	96
1	I	173/189 (92%)	173 (100%)	0	100	100
1	J	179/189 (95%)	179 (100%)	0	100	100
1	K	177/189 (94%)	176 (99%)	1 (1%)	90	96
1	L	172/189 (91%)	172 (100%)	0	100	100
All	All	2101/2268 (93%)	2091 (100%)	10 (0%)	92	97

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	240	VAL
1	F	284	ARG
1	G	115	ARG
1	D	240	VAL
1	F	300	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	H	219	HIS
1	J	112	GLN
1	L	112	GLN

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 ⓘ

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, 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	200/227 (88%)	0.11	2 (1%) 84 88	24, 40, 67, 82	0
1	B	202/227 (88%)	0.05	3 (1%) 76 81	26, 40, 65, 86	0
1	C	203/227 (89%)	-0.05	3 (1%) 76 81	23, 38, 62, 77	0
1	D	200/227 (88%)	-0.14	2 (1%) 84 88	22, 33, 57, 81	0
1	E	197/227 (86%)	-0.18	1 (0%) 91 94	21, 36, 56, 75	0
1	F	204/227 (89%)	-0.05	4 (1%) 68 75	22, 34, 60, 72	0
1	G	203/227 (89%)	-0.15	2 (0%) 84 88	20, 32, 56, 69	0
1	H	199/227 (87%)	0.10	4 (2%) 68 75	25, 40, 62, 77	0
1	I	199/227 (87%)	-0.19	3 (1%) 76 81	17, 34, 55, 75	0
1	J	206/227 (90%)	-0.07	3 (1%) 76 81	21, 32, 59, 90	0
1	K	203/227 (89%)	0.07	3 (1%) 76 81	26, 38, 66, 86	0
1	L	198/227 (87%)	0.29	9 (4%) 37 46	29, 47, 67, 85	0
All	All	2414/2724 (88%)	-0.02	39 (1%) 74 80	17, 37, 63, 90	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	210	THR	10.5
1	K	300	ARG	6.7
1	J	211	VAL	5.2
1	H	209	PRO	4.6
1	J	300	ARG	4.6

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.