



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:06 PM UTC

PDB ID : 4XWS / pdb_00004xws
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (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

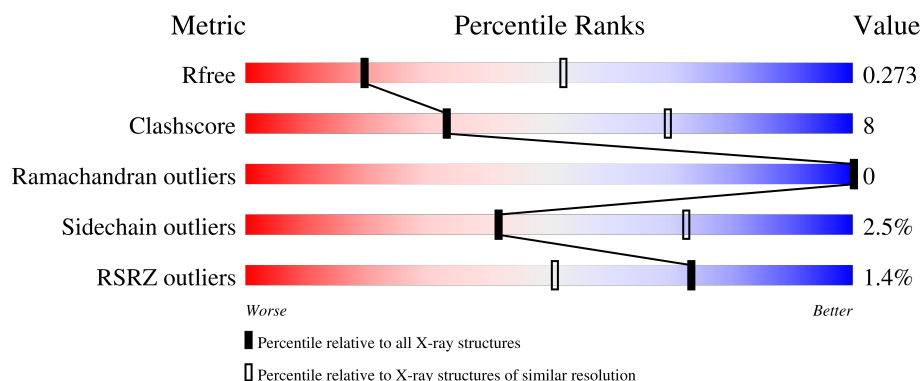
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	0% 75% 18% 7%
1	B	227	0% 64% 20% 15%
1	C	227	2% 65% 16% 16%
1	D	227	0% 72% 14% 15%

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			

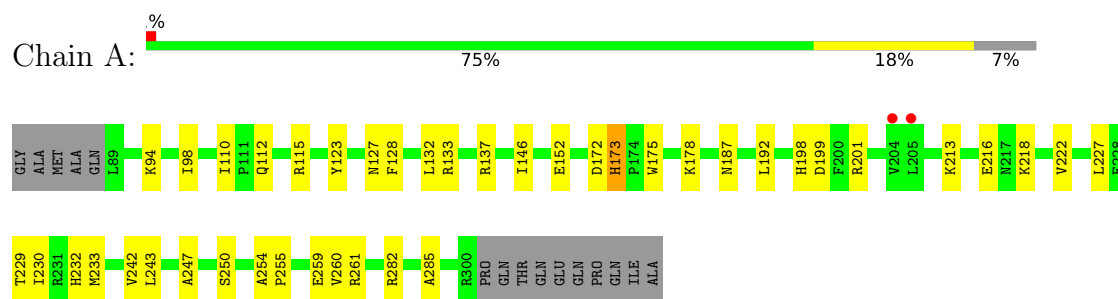
There are 20 discrepancies between the modelled and reference sequences:

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

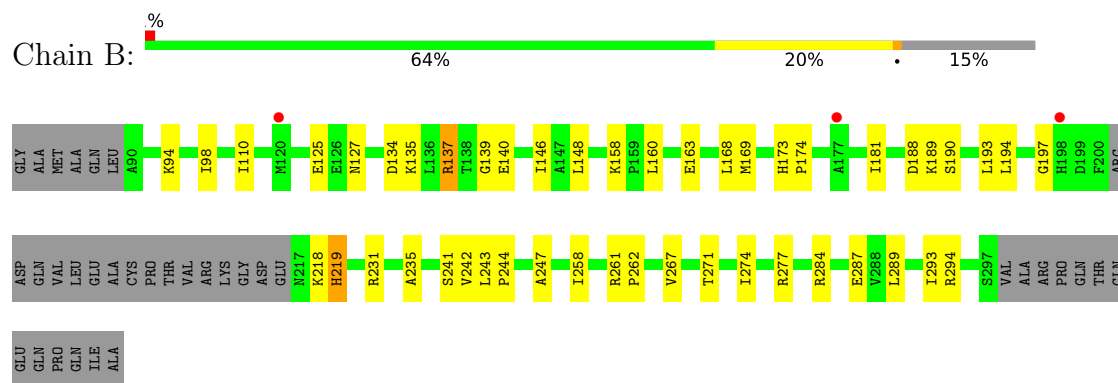
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

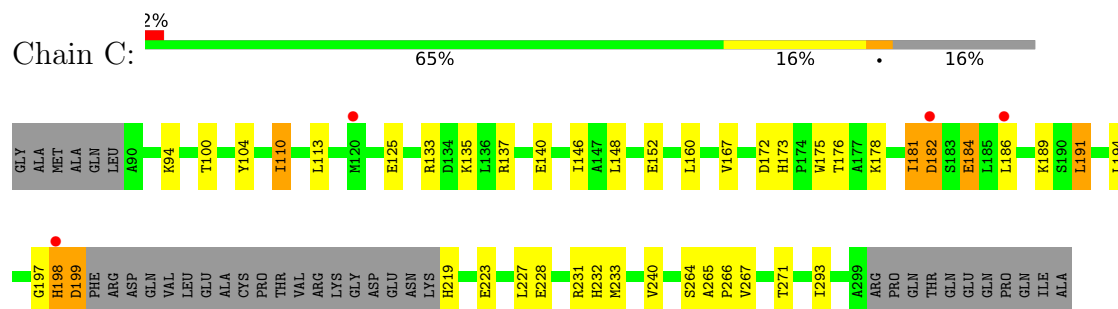
• Molecule 1: OxyR



• Molecule 1: OxyR

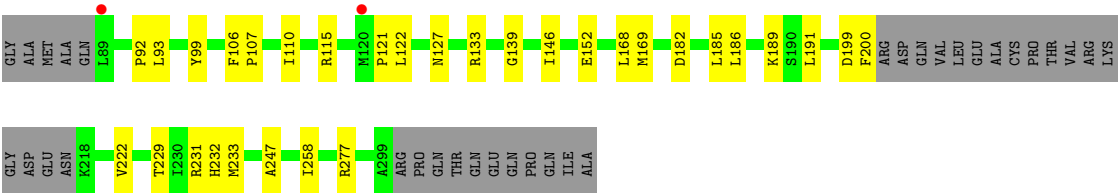


• Molecule 1: OxyR



• Molecule 1: OxyR





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	129.94Å 129.94Å 135.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 3.01 19.99 – 3.01	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.99-3.01) 97.8 (19.99-3.01)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.229 , 0.260 0.238 , 0.273	Depositor DCC
R_{free} test set	2004 reflections (7.73%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.077 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	6176	wwPDB-VP
Average B, all atoms (Å ²)	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 23.83 % 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 4.3128e-03. 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, 0.333 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	0.31	0/1708	0.82	3/2333 (0.1%)
1	B	0.30	0/1550	0.75	0/2118
1	C	0.35	0/1533	0.88	8/2097 (0.4%)
1	D	0.28	0/1562	0.73	0/2135
All	All	0.31	0/6353	0.80	11/8683 (0.1%)

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 (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	198	HIS	N-CA-C	7.76	119.52	111.14
1	A	173	HIS	CA-C-N	6.81	128.35	119.84
1	A	173	HIS	C-N-CA	6.81	128.35	119.84
1	C	181	ILE	CA-C-N	-6.37	111.43	121.87
1	C	181	ILE	C-N-CA	-6.37	111.43	121.87
1	C	197	GLY	N-CA-C	6.15	120.11	112.73
1	C	110	ILE	CB-CA-C	-5.08	108.97	114.35
1	C	265	ALA	CA-C-N	-5.06	113.51	119.84
1	C	265	ALA	C-N-CA	-5.06	113.51	119.84
1	C	267	VAL	N-CA-C	5.05	113.72	109.02
1	A	110	ILE	CB-CA-C	-5.02	109.03	114.35

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	24	0
1	B	1506	0	1515	29	0
1	C	1490	0	1501	30	0
1	D	1518	0	1534	17	0
All	All	6176	0	6227	97	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 8.

All (97) 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:125:GLU:OE2	1:B:135:LYS:NZ	2.24	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:230:ILE:HA	1:A:233:MET:HE3	1.84	0.59
1:D:186:LEU:HD22	1:D:191:LEU:HD13	1.87	0.56
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:A:222:VAL:HG11	1:A:233:MET:HE1	1.91	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:247:ALA:O	1:A:250:SER:OG	2.27	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:229:THR:HG22	1:D:233:MET:HE2	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:A:229:THR:HG22	1:A:233:MET:HE2	1.96	0.47
1:C:198:HIS:CE1	1:C:227:LEU:HD22	2.51	0.46
1:B:169:MET:HE1	1:B:181:ILE:HD11	1.97	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:D:222:VAL:HG21	1:D:233:MET:HE1	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:232:HIS:CG	1:B:110:ILE:HG21	2.53	0.43
1:A:254:ALA:HA	1:A:255:PRO:HD3	1.93	0.43
1:B:289:LEU:O	1:B:293:ILE:HG13	2.18	0.43
1:C:199:ASP:OD1	1:C:199:ASP:C	2.60	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:A:259:GLU:CD	1:A:261:ARG:HH22	2.26	0.42
1:C:94:LYS:HD2	1:C:140:GLU:O	2.19	0.42
1:C:184:GLU:H	1:C:184:GLU:CD	2.28	0.42
1:A:227:LEU:HD13	1:A:243:LEU:HD22	2.02	0.42
1:D:115:ARG:HE	1:D:115:ARG:HB2	1.65	0.41
1:C:233:MET:HE3	1:C:233:MET:HB2	1.89	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:D:169:MET:HE2	1:D:169:MET:HB3	1.87	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:HA	1:B:189:LYS:HD3	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%)	178 (98%)	4 (2%)	45	74
1	B	165/193 (86%)	161 (98%)	4 (2%)	43	73
1	C	163/193 (84%)	156 (96%)	7 (4%)	26	60
1	D	166/193 (86%)	164 (99%)	2 (1%)	63	82
All	All	676/772 (88%)	659 (98%)	17 (2%)	42	72

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ILE
1	A	192	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	213	LYS
1	A	260	VAL
1	B	137	ARG
1	B	146	ILE
1	B	219	HIS
1	B	267	VAL
1	C	113	LEU
1	C	146	ILE
1	C	172	ASP
1	C	184	GLU
1	C	191	LEU
1	C	199	ASP
1	C	223	GLU
1	D	146	ILE
1	D	189	LYS

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

Mol	Chain	Res	Type
1	B	173	HIS
1	C	108	HIS
1	C	198	HIS
1	D	187	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](#)

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, 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	212/227 (93%)	0.07	2 (0%) 81 61	36, 61, 105, 138	0
1	B	192/227 (84%)	-0.05	3 (1%) 70 47	38, 55, 84, 104	0
1	C	191/227 (84%)	0.16	4 (2%) 63 40	33, 62, 107, 122	0
1	D	194/227 (85%)	-0.27	2 (1%) 79 59	34, 49, 69, 78	0
All	All	789/908 (86%)	-0.02	11 (1%) 73 51	33, 56, 99, 138	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	LEU	3.9
1	A	204	VAL	3.6
1	B	198	HIS	3.1
1	C	198	HIS	2.8
1	C	186	LEU	2.4
1	C	120	MET	2.3
1	C	182	ASP	2.2
1	B	177	ALA	2.1
1	D	89	LEU	2.1
1	B	120	MET	2.1
1	D	120	MET	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 oligosaccharides 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.