



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:39 PM GMT

PDB ID : 3UKI
Title : Crystal structure of reduced OxyR from Porphyromonas gingivalis
Authors : Svintradze, D.V.; Wright, H.T.; Collazo-Santiago, E.A.; Lewis, J.P.
Deposited on : 2011-11-09
Resolution : 4.15 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
<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

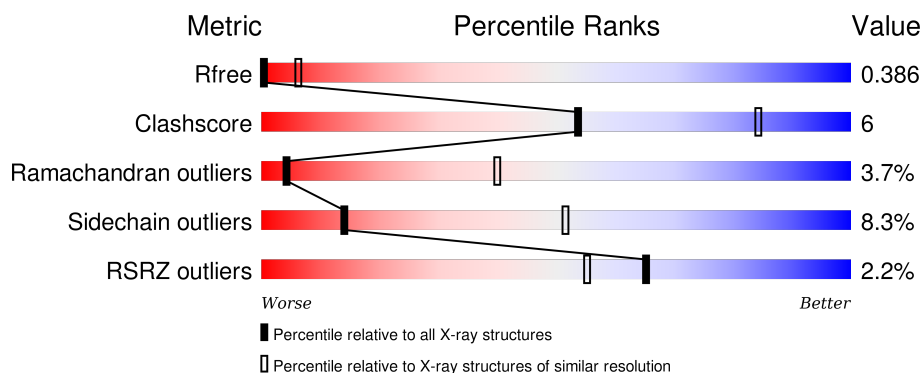
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.15 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	1029 (4.72-3.60)
Clashscore	102246	1128 (4.72-3.60)
Ramachandran outliers	100387	1074 (4.72-3.60)
Sidechain outliers	100360	1060 (4.72-3.60)
RSRZ outliers	91569	1033 (4.72-3.60)

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	223	
1	B	223	
1	C	223	
1	D	223	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11888 atoms, of which 5782 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	207	Total	C	H	N	O	S	0	0	0
			2972	979	1445	259	280	9			
1	B	204	Total	C	H	N	O	S	0	0	0
			3060	993	1504	268	286	9			
1	C	208	Total	C	H	N	O	S	0	0	0
			3092	1003	1517	269	294	9			
1	D	204	Total	C	H	N	O	S	0	0	0
			2764	918	1316	253	269	8			

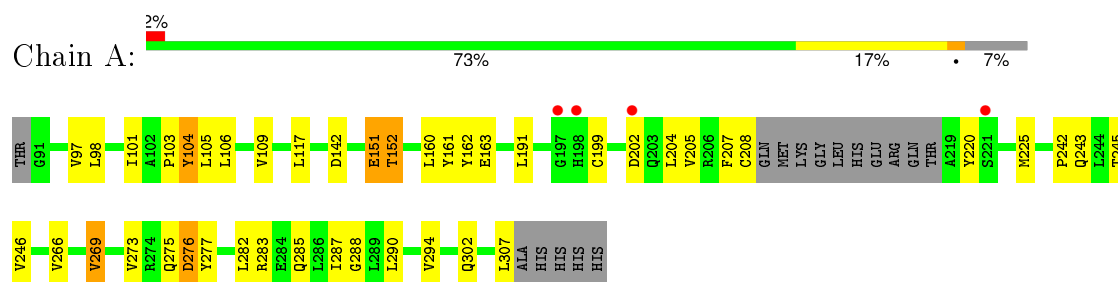
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	HIS	-	EXPRESSION TAG	UNP Q20K61
A	310	HIS	-	EXPRESSION TAG	UNP Q20K61
A	311	HIS	-	EXPRESSION TAG	UNP Q20K61
A	312	HIS	-	EXPRESSION TAG	UNP Q20K61
B	309	HIS	-	EXPRESSION TAG	UNP Q20K61
B	310	HIS	-	EXPRESSION TAG	UNP Q20K61
B	311	HIS	-	EXPRESSION TAG	UNP Q20K61
B	312	HIS	-	EXPRESSION TAG	UNP Q20K61
C	309	HIS	-	EXPRESSION TAG	UNP Q20K61
C	310	HIS	-	EXPRESSION TAG	UNP Q20K61
C	311	HIS	-	EXPRESSION TAG	UNP Q20K61
C	312	HIS	-	EXPRESSION TAG	UNP Q20K61
D	309	HIS	-	EXPRESSION TAG	UNP Q20K61
D	310	HIS	-	EXPRESSION TAG	UNP Q20K61
D	311	HIS	-	EXPRESSION TAG	UNP Q20K61
D	312	HIS	-	EXPRESSION TAG	UNP Q20K61

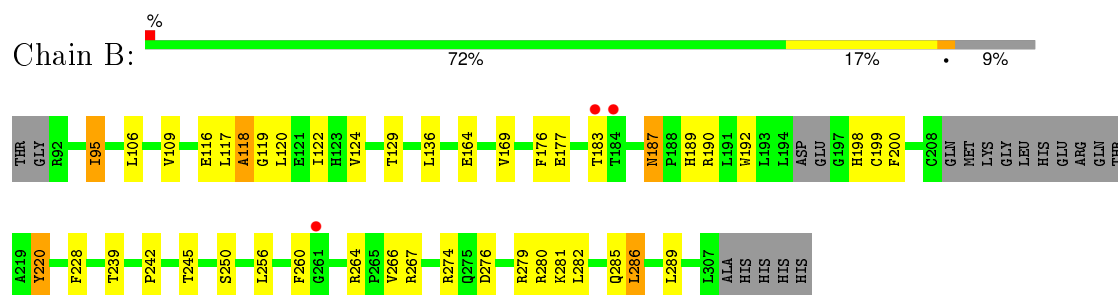
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

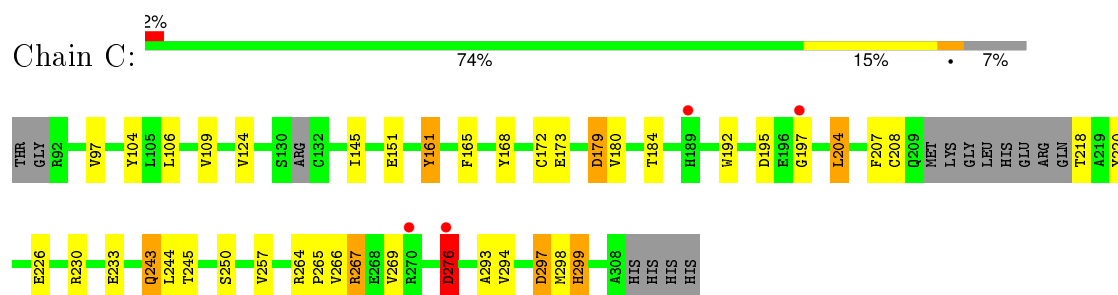
• Molecule 1: OxyR



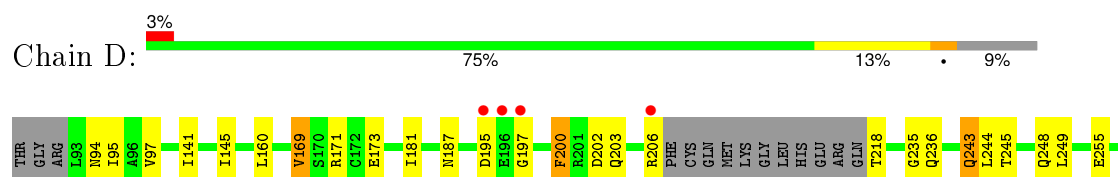
• Molecule 1: OxyR

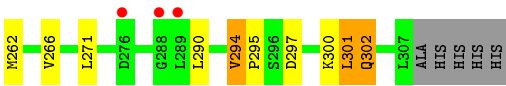


• Molecule 1: OxyR



• Molecule 1: OxyR





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.24Å 82.81Å 170.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.65 – 4.15 21.76 – 4.15	Depositor EDS
% Data completeness (in resolution range)	96.4 (21.65-4.15) 96.8 (21.76-4.15)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 4.22Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.309 , 0.405 0.303 , 0.386	Depositor DCC
R_{free} test set	687 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	98.4	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 98.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	2 of 6904 reflections (0.029%)	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	11888	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.35	0/1558	0.68	0/2124
1	B	0.31	0/1586	0.65	0/2156
1	C	0.32	0/1604	0.67	0/2181
1	D	0.31	0/1475	0.65	1/2012 (0.0%)
All	All	0.33	0/6223	0.66	1/8473 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	206	ARG	NE-CZ-NH1	5.11	122.85	120.30

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	1527	1445	1441	25	0
1	B	1556	1504	1500	19	0
1	C	1575	1517	1513	21	0
1	D	1448	1316	1312	13	0
All	All	6106	5782	5766	77	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.

All (77) 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:D:294:VAL:HG12	1:D:295:PRO:HD2	1.67	0.76
1:B:279:ARG:O	1:B:281:LYS:N	2.17	0.76
1:D:243:GLN:O	1:D:245:THR:N	2.21	0.73
1:A:243:GLN:O	1:A:246:VAL:HG22	1.91	0.71
1:C:106:LEU:CD1	1:C:124:VAL:HG11	2.24	0.68
1:A:204:LEU:O	1:A:208:CYS:N	2.26	0.68
1:C:243:GLN:O	1:C:245:THR:N	2.30	0.64
1:C:106:LEU:HD13	1:C:124:VAL:HG11	1.79	0.64
1:D:202:ASP:OD1	1:D:203:GLN:N	2.31	0.63
1:C:297:ASP:O	1:C:299:HIS:N	2.32	0.62
1:B:117:LEU:HD11	1:B:289:LEU:CD1	2.31	0.61
1:B:136:LEU:O	1:B:274:ARG:NH1	2.34	0.61
1:B:106:LEU:HA	1:B:109:VAL:HG12	1.84	0.60
1:C:109:VAL:HG12	1:C:293:ALA:CB	2.31	0.59
1:B:106:LEU:HD11	1:B:124:VAL:HG11	1.85	0.58
1:A:142:ASP:O	1:A:273:VAL:HG23	2.04	0.58
1:A:97:VAL:HG21	1:A:106:LEU:HD21	1.86	0.57
1:C:168:TYR:CD1	1:C:257:VAL:HG12	2.40	0.56
1:B:106:LEU:CD1	1:B:124:VAL:HG11	2.37	0.55
1:C:97:VAL:HG13	1:C:145:ILE:HB	1.89	0.54
1:A:163:GLU:OE1	1:A:242:PRO:HB2	2.09	0.53
1:C:179:ASP:O	1:C:180:VAL:HG23	2.10	0.52
1:A:104:TYR:CZ	1:A:245:THR:HG22	2.46	0.51
1:B:187:ASN:OD1	1:B:189:HIS:NE2	2.44	0.51
1:C:226:GLU:OE1	1:C:230:ARG:NH1	2.43	0.50
1:B:117:LEU:HD11	1:B:289:LEU:HD11	1.94	0.50
1:C:267:ARG:HD2	1:C:269:VAL:HG23	1.94	0.50
1:D:200:PHE:N	1:D:200:PHE:CD2	2.80	0.49
1:A:103:PRO:HG2	1:A:104:TYR:CE1	2.47	0.49
1:A:104:TYR:CE1	1:A:245:THR:HG22	2.47	0.49
1:A:161:TYR:CE1	1:A:294:VAL:HG11	2.47	0.49
1:C:161:TYR:CE1	1:C:294:VAL:HG11	2.47	0.49
1:B:120:LEU:O	1:B:122:ILE:N	2.46	0.48
1:A:101:ILE:HD11	1:A:269:VAL:HG22	1.95	0.47
1:A:287:ILE:HG13	1:A:288:GLY:N	2.29	0.47
1:B:192:TRP:HB3	1:B:228:PHE:CD2	2.50	0.47
1:C:184:THR:O	1:C:184:THR:OG1	2.29	0.47
1:D:271:LEU:HD11	1:D:290:LEU:HD23	1.96	0.47
1:B:242:PRO:O	1:B:245:THR:OG1	2.24	0.47
1:D:169:VAL:HG23	1:D:173:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:ARG:NH2	1:D:255:GLU:OE1	2.48	0.47
1:C:266:VAL:HG22	1:C:267:ARG:O	2.15	0.46
1:C:233:GLU:OE1	1:D:248:GLN:NE2	2.49	0.46
1:A:105:LEU:HD13	1:A:109:VAL:HG13	1.98	0.46
1:C:106:LEU:HD11	1:C:124:VAL:HG11	1.98	0.45
1:C:276:ASP:OD1	1:C:276:ASP:N	2.50	0.45
1:C:168:TYR:HD1	1:C:257:VAL:HG12	1.81	0.44
1:A:275:GLN:O	1:A:277:TYR:N	2.50	0.44
1:C:165:PHE:CD1	1:C:204:LEU:CD2	3.01	0.44
1:A:160:LEU:CB	1:A:269:VAL:HG12	2.48	0.44
1:D:160:LEU:HD11	1:D:271:LEU:CD1	2.48	0.44
1:B:95:ILE:HD13	1:B:286:LEU:HD21	2.00	0.43
1:A:160:LEU:HB2	1:A:269:VAL:HG12	2.00	0.43
1:A:97:VAL:HG12	1:A:101:ILE:HB	2.00	0.43
1:B:282:LEU:O	1:B:285:GLN:N	2.52	0.42
1:B:117:LEU:O	1:B:118:ALA:HB3	2.19	0.42
1:D:95:ILE:HD12	1:D:145:ILE:CD1	2.49	0.42
1:D:181:ILE:O	1:D:181:ILE:HG13	2.20	0.42
1:C:104:TYR:CD1	1:C:245:THR:HG22	2.54	0.42
1:B:169:VAL:O	1:B:256:LEU:CD1	2.68	0.42
1:A:160:LEU:HD11	1:A:290:LEU:HB2	2.02	0.41
1:A:282:LEU:O	1:A:285:GLN:N	2.53	0.41
1:A:162:TYR:HB3	1:A:266:VAL:HG11	2.00	0.41
1:A:225:MET:CE	1:A:242:PRO:HD2	2.50	0.41
1:A:160:LEU:CD1	1:A:290:LEU:HB2	2.51	0.41
1:A:151:GLU:O	1:A:152:THR:CB	2.69	0.41
1:A:101:ILE:CD1	1:A:269:VAL:HG22	2.50	0.41
1:C:168:TYR:CE1	1:C:257:VAL:HG12	2.56	0.41
1:B:117:LEU:CD1	1:B:289:LEU:CD1	2.99	0.41
1:B:282:LEU:HD21	1:B:286:LEU:HD23	2.03	0.41
1:B:266:VAL:HG22	1:B:267:ARG:O	2.21	0.41
1:C:207:PHE:CG	1:C:265:PRO:HG3	2.56	0.40
1:D:301:LEU:O	1:D:302:GLN:CB	2.69	0.40
1:A:104:TYR:CD1	1:A:104:TYR:N	2.85	0.40
1:A:199:CYS:HA	1:A:202:ASP:HB3	2.04	0.40
1:D:294:VAL:HG12	1:D:295:PRO:CD	2.42	0.40
1:B:164:GLU:HA	1:B:266:VAL:HG23	2.03	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	203/223 (91%)	182 (90%)	17 (8%)	4 (2%)	9	53
1	B	198/223 (89%)	177 (89%)	14 (7%)	7 (4%)	4	41
1	C	202/223 (91%)	174 (86%)	19 (9%)	9 (4%)	3	34
1	D	200/223 (90%)	173 (86%)	17 (8%)	10 (5%)	3	32
All	All	803/892 (90%)	706 (88%)	67 (8%)	30 (4%)	4	40

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	THR
1	A	276	ASP
1	B	119	GLY
1	B	199	CYS
1	B	280	ARG
1	C	195	ASP
1	C	243	GLN
1	C	244	LEU
1	C	276	ASP
1	C	297	ASP
1	C	298	MET
1	D	244	LEU
1	D	297	ASP
1	A	151	GLU
1	B	276	ASP
1	C	208	CYS
1	D	301	LEU
1	A	302	GLN
1	B	200	PHE
1	C	197	GLY
1	C	220	TYR
1	D	195	ASP

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Mol	Chain	Res	Type
1	D	197	GLY
1	D	243	GLN
1	D	300	LYS
1	B	118	ALA
1	D	187	ASN
1	D	235	GLY
1	D	302	GLN
1	B	220	TYR

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	151/197 (77%)	140 (93%)	11 (7%)	17	57
1	B	160/197 (81%)	145 (91%)	15 (9%)	11	45
1	C	162/197 (82%)	149 (92%)	13 (8%)	15	53
1	D	132/197 (67%)	121 (92%)	11 (8%)	14	51
All	All	605/788 (77%)	555 (92%)	50 (8%)	14	51

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	LEU
1	A	104	TYR
1	A	117	LEU
1	A	191	LEU
1	A	205	VAL
1	A	207	PHE
1	A	220	TYR
1	A	269	VAL
1	A	276	ASP
1	A	283	ARG
1	A	307	LEU
1	B	95	ILE
1	B	116	GLU

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Mol	Chain	Res	Type
1	B	129	THR
1	B	176	PHE
1	B	177	GLU
1	B	183	THR
1	B	187	ASN
1	B	190	ARG
1	B	198	HIS
1	B	220	TYR
1	B	239	THR
1	B	250	SER
1	B	260	PHE
1	B	264	ARG
1	B	286	LEU
1	C	151	GLU
1	C	161	TYR
1	C	172	CYS
1	C	173	GLU
1	C	179	ASP
1	C	192	TRP
1	C	204	LEU
1	C	218	THR
1	C	250	SER
1	C	264	ARG
1	C	267	ARG
1	C	276	ASP
1	C	299	HIS
1	D	94	ASN
1	D	97	VAL
1	D	141	ILE
1	D	169	VAL
1	D	200	PHE
1	D	218	THR
1	D	236	GLN
1	D	249	LEU
1	D	262	MET
1	D	266	VAL
1	D	294	VAL

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	123	HIS

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Mol	Chain	Res	Type
1	D	198	HIS

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](#)

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	207/223 (92%)	0.11	4 (1%) 70 60	44, 98, 156, 227	0
1	B	204/223 (91%)	0.05	3 (1%) 76 67	48, 90, 148, 223	0
1	C	208/223 (93%)	0.12	4 (1%) 70 60	59, 98, 165, 255	0
1	D	204/223 (91%)	0.24	7 (3%) 49 38	71, 112, 175, 232	0
All	All	823/892 (92%)	0.13	18 (2%) 65 55	44, 99, 165, 255	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	197	GLY	5.4
1	D	196	GLU	3.8
1	D	195	ASP	3.5
1	B	261	GLY	3.2
1	B	184	THR	2.9
1	A	198	HIS	2.8
1	A	202	ASP	2.7
1	C	197	GLY	2.7
1	A	221	SER	2.7
1	C	189	HIS	2.6
1	D	276	ASP	2.4
1	D	288	GLY	2.4
1	A	197	GLY	2.3
1	D	206	ARG	2.1
1	C	270	ARG	2.1
1	D	289	LEU	2.1
1	C	276	ASP	2.0
1	B	183	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.