



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:27 AM GMT

PDB ID : 2QSG
Title : Crystal structure of Rad4-Rad23 bound to a UV-damaged DNA
Authors : Min, J.-H.; Pavletich, N.P.
Deposited on : 2007-07-31
Resolution : 3.10 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

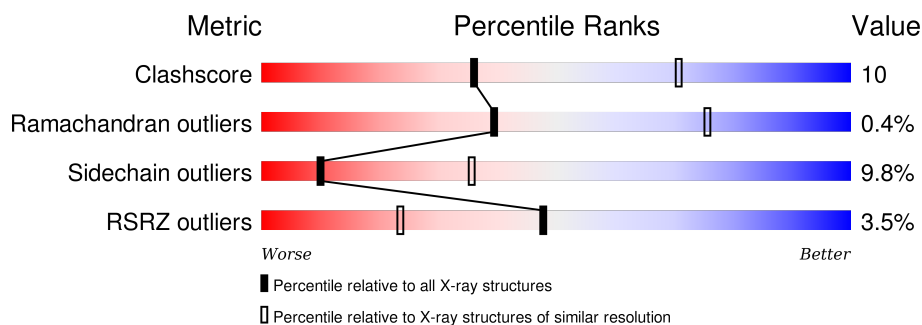
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	W	24	
2	Y	24	
3	A	533	
4	X	171	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5480 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 DNA chain called native strand of the CPD-mismatch DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	W	24	Total	C	N	O	P	0	0	0
			481	233	82	143	23			

- Molecule 2 is a DNA chain called damaged strand of the CPD-mismatch DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	22	Total	C	N	O	P	0	0	0
			451	218	82	131	20			

- Molecule 3 is a protein called DNA repair protein RAD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	502	Total	C	N	O	S	0	0	0
			4132	2633	744	728	27			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	MET	-	INITIATING METHIONINE	UNP P14736
A	223	GLU	VAL	SEE REMARK 999	UNP P14736
A	225	LEU	ILE	SEE REMARK 999	UNP P14736

- Molecule 4 is a protein called UV excision repair protein RAD23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	X	54	Total	C	N	O	S	0	0	0
			416	265	70	79	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	228	GLY	-	EXPRESSION TAG	UNP P32628

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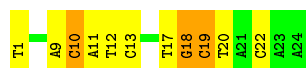
Chain	Residue	Modelled	Actual	Comment	Reference
X	229	SER	-	EXPRESSION TAG	UNP P32628

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 ($RSRZ > 2$). 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.

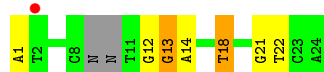
- Molecule 1: native strand of the CPD-mismatch DNA

Chain W: 



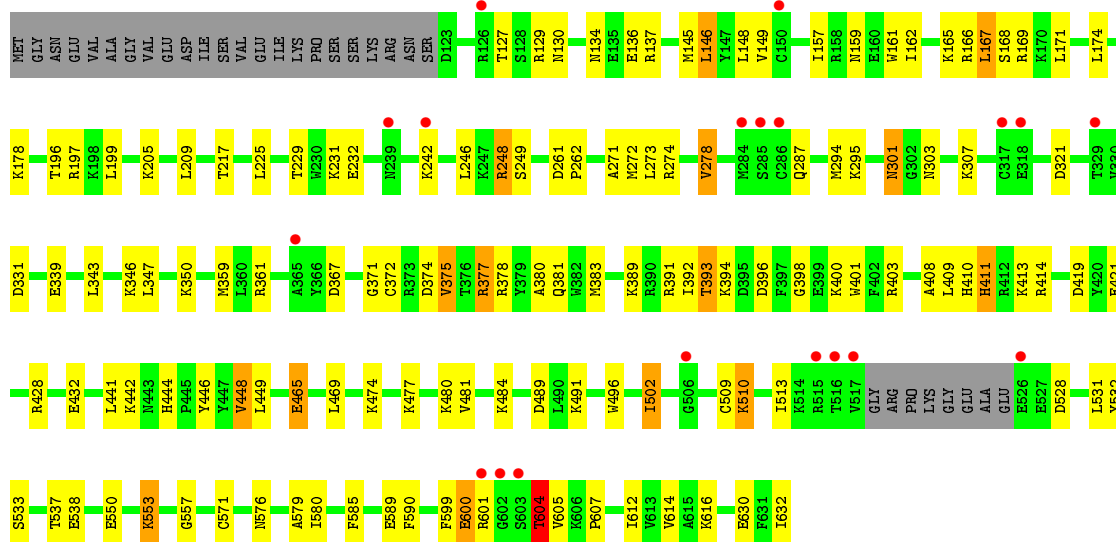
- Molecule 2: damaged strand of the CPD-mismatch DNA

Chain Y: 



- Molecule 3: DNA repair protein RAD4

Chain A: 



- Molecule 4: UV excision repair protein RAD23

Chain X: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	79.64Å 79.64Å 403.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 29.11 – 3.05	Depositor EDS
% Data completeness (in resolution range)	93.4 (30.00-3.10) 92.6 (29.11-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 3.05Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.246 , 0.277 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	83.4	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 14.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 24856 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5480	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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	W	0.73	0/537	1.52	9/825 (1.1%)
2	Y	0.72	0/505	1.53	9/778 (1.2%)
3	A	0.38	0/4221	0.54	0/5673
4	X	0.37	0/422	0.55	0/575
All	All	0.46	0/5685	0.84	18/7851 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	12	DG	O4'-C1'-N9	8.96	114.28	108.00
1	W	19	DC	O4'-C1'-N1	8.27	113.79	108.00
2	Y	13	DG	P-O3'-C3'	7.08	128.19	119.70
1	W	22	DC	O4'-C1'-N1	6.84	112.79	108.00
2	Y	21	DG	O4'-C1'-N9	6.83	112.78	108.00
1	W	18	DG	P-O3'-C3'	6.80	127.86	119.70
1	W	12	DT	P-O3'-C3'	6.47	127.46	119.70
1	W	22	DC	C1'-O4'-C4'	-6.35	103.75	110.10
2	Y	1	DA	P-O3'-C3'	6.24	127.19	119.70
2	Y	18	DT	C1'-O4'-C4'	-6.01	104.08	110.10
2	Y	12	DG	C1'-O4'-C4'	-5.85	104.25	110.10
2	Y	18	DT	O4'-C1'-N1	5.77	112.04	108.00
2	Y	18	DT	O4'-C4'-C3'	-5.77	102.19	104.50
1	W	1	DT	C6-C5-C7	-5.66	119.50	122.90
1	W	10	DC	O4'-C1'-N1	5.58	111.90	108.00
2	Y	22	DT	O4'-C1'-N1	5.54	111.88	108.00
1	W	13	DC	P-O3'-C3'	5.18	125.92	119.70
1	W	19	DC	P-O3'-C3'	5.09	125.81	119.70

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	W	481	0	274	8	0
2	Y	451	0	254	2	0
3	A	4132	0	4214	89	0
4	X	416	0	427	12	0
All	All	5480	0	5169	102	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 10.

All (102) 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)
3:A:159:ASN:HD21	3:A:274:ARG:HH22	1.19	0.90
3:A:444:HIS:HD2	3:A:446:TYR:H	1.29	0.80
3:A:580:ILE:HA	3:A:612:ILE:HD11	1.66	0.78
3:A:599:PHE:O	3:A:600:GLU:HG2	1.85	0.76
1:W:18:DG:OP1	1:W:18:DG:H4'	1.89	0.72
3:A:444:HIS:CD2	3:A:446:TYR:H	2.09	0.71
3:A:465:GLU:HG2	3:A:480:LYS:HB3	1.75	0.69
3:A:448:VAL:HG22	3:A:484:LYS:HG2	1.76	0.67
3:A:377:ARG:HD3	3:A:377:ARG:O	1.97	0.65
4:X:265:LEU:HD22	4:X:305:LEU:HD21	1.80	0.64
3:A:550:GLU:HA	3:A:589:GLU:HG2	1.80	0.63
1:W:10:DC:H2'	1:W:11:DA:C8	2.34	0.63
3:A:604:THR:HG22	3:A:605:VAL:H	1.64	0.63
3:A:273:LEU:HB3	3:A:278:VAL:HG22	1.81	0.62
4:X:266:ARG:HD3	4:X:309:VAL:HG23	1.82	0.62
3:A:159:ASN:ND2	3:A:274:ARG:HH22	1.96	0.61
3:A:130:ASN:O	3:A:295:LYS:HA	2.00	0.61
3:A:145:MET:O	3:A:149:VAL:HG23	2.01	0.60
3:A:229:THR:OG1	3:A:232:GLU:HG3	2.01	0.59
3:A:414:ARG:NH1	3:A:419:ASP:OD1	2.35	0.59
3:A:380:ALA:HB3	3:A:383:MET:HG2	1.83	0.59
3:A:571:CYS:O	3:A:616:LYS:HE3	2.03	0.58
3:A:377:ARG:NH2	3:A:432:GLU:OE2	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:287:GLN:NE2	3:A:359:MET:H	2.02	0.58
3:A:372:CYS:H	3:A:410:HIS:HD2	1.54	0.56
3:A:502:ILE:HD12	3:A:538:GLU:HB3	1.86	0.56
3:A:374:ASP:OD1	3:A:391:ARG:NH2	2.39	0.55
3:A:391:ARG:C	3:A:393:THR:H	2.11	0.54
3:A:448:VAL:CG2	3:A:484:LYS:HG2	2.38	0.53
3:A:580:ILE:H	3:A:580:ILE:HD12	1.72	0.53
3:A:367:ASP:OD2	3:A:371:GLY:HA3	2.09	0.53
3:A:372:CYS:N	3:A:410:HIS:HD2	2.07	0.53
3:A:401:TRP:NE1	4:X:298:PRO:HG3	2.23	0.53
1:W:11:DA:H3'	3:A:134:ASN:ND2	2.25	0.51
1:W:10:DC:H2'	1:W:11:DA:H8	1.75	0.51
1:W:10:DC:H2''	1:W:11:DA:O5'	2.10	0.51
3:A:159:ASN:HD21	3:A:274:ARG:NH2	1.99	0.51
3:A:599:PHE:O	3:A:600:GLU:CG	2.57	0.50
3:A:600:GLU:HG3	3:A:601:ARG:HH21	1.77	0.49
3:A:375:VAL:CG2	3:A:378:ARG:HH21	2.26	0.49
3:A:396:ASP:O	3:A:400:LYS:HG2	2.12	0.49
3:A:196:THR:HG23	3:A:321:ASP:OD1	2.13	0.49
3:A:378:ARG:NH2	3:A:421:GLU:OE2	2.46	0.48
3:A:509:CYS:HB3	3:A:532:TYR:CZ	2.48	0.48
3:A:161:TRP:CE2	3:A:248:ARG:HG3	2.47	0.48
3:A:600:GLU:HB3	3:A:601:ARG:NE	2.28	0.48
3:A:287:GLN:HE22	3:A:359:MET:N	2.11	0.48
3:A:600:GLU:CB	3:A:601:ARG:NH2	2.77	0.47
3:A:287:GLN:HE22	3:A:359:MET:H	1.61	0.47
3:A:600:GLU:HB3	3:A:601:ARG:H	1.52	0.47
1:W:9:DA:H2''	1:W:10:DC:H5''	1.96	0.47
2:Y:13:DG:H2''	2:Y:14:DA:OP2	2.14	0.47
3:A:273:LEU:HB3	3:A:278:VAL:CG2	2.44	0.46
3:A:509:CYS:HB2	3:A:531:LEU:O	2.15	0.46
3:A:174:LEU:CB	3:A:272:MET:HE2	2.46	0.46
3:A:599:PHE:O	3:A:600:GLU:CB	2.62	0.45
3:A:590:PHE:CD1	3:A:612:ILE:HD12	2.51	0.45
3:A:585:PHE:CD2	3:A:632:ILE:HG23	2.51	0.45
3:A:287:GLN:NE2	3:A:359:MET:N	2.64	0.45
1:W:17:DT:C2	3:A:607:PRO:HG3	2.52	0.45
3:A:205:LYS:O	3:A:209:LEU:HG	2.18	0.44
4:X:289:GLN:H	4:X:289:GLN:CD	2.21	0.44
3:A:301:ASN:HD22	3:A:303:ASN:H	1.65	0.44
4:X:282:ASN:HD21	4:X:286:ARG:HH21	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:449:LEU:HD23	3:A:481:VAL:HG22	1.99	0.43
3:A:377:ARG:HD2	3:A:428:ARG:CB	2.48	0.43
3:A:580:ILE:HG13	3:A:612:ILE:HD11	2.00	0.43
4:X:262:LEU:HD21	4:X:266:ARG:HH22	1.83	0.43
3:A:513:ILE:HD13	3:A:531:LEU:CD1	2.48	0.43
3:A:261:ASP:HB2	3:A:262:PRO:HD2	1.99	0.43
3:A:585:PHE:CG	3:A:632:ILE:HG12	2.54	0.43
3:A:157:ILE:HG21	4:X:270:SER:HB2	2.00	0.43
3:A:510:LYS:HD3	3:A:533:SER:HB3	2.00	0.42
3:A:377:ARG:HD3	3:A:377:ARG:C	2.39	0.42
3:A:401:TRP:CD1	4:X:298:PRO:HG3	2.54	0.42
3:A:391:ARG:C	3:A:393:THR:N	2.73	0.42
3:A:339:GLU:OE1	3:A:346:LYS:HG3	2.20	0.42
3:A:474:LYS:HB2	3:A:477:LYS:HD2	2.02	0.42
3:A:465:GLU:CD	3:A:465:GLU:H	2.22	0.42
3:A:391:ARG:O	3:A:394:LYS:HG2	2.19	0.42
3:A:389:LYS:O	3:A:394:LYS:HE3	2.20	0.42
3:A:146:LEU:HD22	4:X:280:LEU:HD22	2.02	0.42
2:Y:18:DT:H5'	3:A:137:ARG:HH12	1.84	0.42
3:A:576:ASN:HB3	3:A:579:ALA:HB2	2.02	0.41
3:A:491:LYS:HB2	3:A:496:TRP:CE2	2.55	0.41
3:A:145:MET:HG2	3:A:392:ILE:HG12	2.02	0.41
3:A:392:ILE:O	3:A:398:GLY:HA3	2.20	0.41
3:A:496:TRP:CD2	3:A:537:THR:HG21	2.55	0.41
3:A:167:LEU:HD22	3:A:171:LEU:HG	2.02	0.41
3:A:377:ARG:HD2	3:A:428:ARG:HB3	2.03	0.41
3:A:225:LEU:HD21	4:X:273:PRO:HG2	2.02	0.41
3:A:162:ILE:HG23	3:A:271:ALA:HA	2.03	0.41
3:A:553:LYS:HG3	3:A:557:GLY:HA2	2.03	0.41
3:A:331:ASP:HB2	3:A:347:LEU:HD21	2.03	0.41
1:W:19:DC:H2''	1:W:20:DT:OP2	2.21	0.41
3:A:408:ALA:O	3:A:411:HIS:HE1	2.04	0.41
3:A:413:LYS:HA	3:A:413:LYS:HD3	1.90	0.41
3:A:513:ILE:HD13	3:A:531:LEU:HD11	2.03	0.40
3:A:261:ASP:HB2	3:A:262:PRO:CD	2.51	0.40
3:A:580:ILE:CA	3:A:612:ILE:HD11	2.42	0.40
4:X:257:LEU:HA	4:X:287:TYR:HE2	1.85	0.40
3:A:246:LEU:H	4:X:272:ASN:HD21	1.68	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	
3	A	498/533 (93%)	460 (92%)	36 (7%)	2 (0%)	39	75
4	X	52/171 (30%)	46 (88%)	6 (12%)	0	100	100
All	All	550/704 (78%)	506 (92%)	42 (8%)	2 (0%)	39	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	600	GLU
3	A	604	THR

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	
3	A	452/477 (95%)	407 (90%)	45 (10%)	9	34
4	X	47/129 (36%)	43 (92%)	4 (8%)	13	45
All	All	499/606 (82%)	450 (90%)	49 (10%)	10	36

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	127	THR
3	A	129	ARG
3	A	136	GLU
3	A	146	LEU

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Mol	Chain	Res	Type
3	A	148	LEU
3	A	165	LYS
3	A	166	ARG
3	A	167	LEU
3	A	168	SER
3	A	169	ARG
3	A	178	LYS
3	A	197	ARG
3	A	199	LEU
3	A	217	THR
3	A	231	LYS
3	A	242	LYS
3	A	248	ARG
3	A	249	SER
3	A	278	VAL
3	A	294	MET
3	A	301	ASN
3	A	307	LYS
3	A	343	LEU
3	A	350	LYS
3	A	361	ARG
3	A	375	VAL
3	A	377	ARG
3	A	381	GLN
3	A	393	THR
3	A	403	ARG
3	A	409	LEU
3	A	411	HIS
3	A	441	LEU
3	A	442	LYS
3	A	448	VAL
3	A	465	GLU
3	A	469	LEU
3	A	489	ASP
3	A	502	ILE
3	A	510	LYS
3	A	528	ASP
3	A	553	LYS
3	A	604	THR
3	A	614	VAL
3	A	630	GLU
4	X	265	LEU

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Mol	Chain	Res	Type
4	X	299	GLU
4	X	307	GLU
4	X	309	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	154	HIS
3	A	159	ASN
3	A	173	ASN
3	A	211	GLN
3	A	267	GLN
3	A	287	GLN
3	A	301	ASN
3	A	303	ASN
3	A	410	HIS
3	A	427	GLN
3	A	444	HIS
4	X	267	GLN
4	X	272	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 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	W	24/24 (100%)	0.03	0 100 100	55, 70, 78, 99	0
2	Y	22/24 (91%)	0.14	1 (4%) 37 17	56, 72, 85, 107	0
3	A	502/533 (94%)	0.03	19 (3%) 44 21	58, 65, 80, 108	0
4	X	54/171 (31%)	-0.33	1 (1%) 70 48	58, 65, 77, 84	0
All	All	602/752 (80%)	0.00	21 (3%) 48 23	55, 66, 81, 108	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	517	VAL	4.4
3	A	317	CYS	4.2
3	A	516	THR	4.1
3	A	526	GLU	3.2
3	A	284	MET	2.9
3	A	602	GLY	2.9
3	A	329	THR	2.7
4	X	309	VAL	2.7
3	A	286	CYS	2.6
3	A	318	GLU	2.6
3	A	285	SER	2.5
3	A	603	SER	2.5
3	A	150	CYS	2.4
3	A	239	ASN	2.3
3	A	242	LYS	2.2
2	Y	2	DT	2.2
3	A	506	GLY	2.2
3	A	601	ARG	2.2
3	A	365	ALA	2.1
3	A	515	ARG	2.1
3	A	126	ARG	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.