



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2025 – 10:45 PM EDT

PDB ID : 2QSG / pdb_00002qsg
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

<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 Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

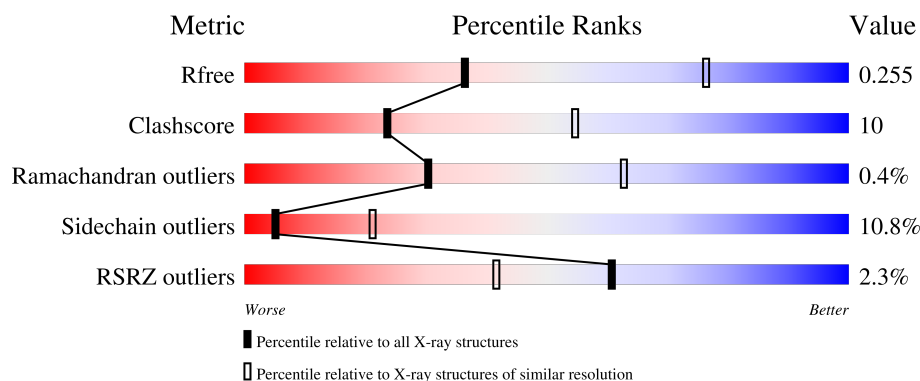
1 Overall quality at a glance

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))
R_{free}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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	W	24	
2	Y	24	
3	A	533	
4	X	171	

2 Entry composition

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

Continued on next page...

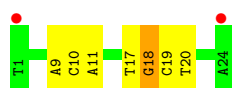
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
X	229	SER	-	expression tag	UNP P32628

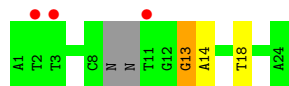
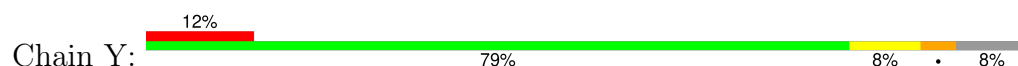
3 Residue-property plots

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.

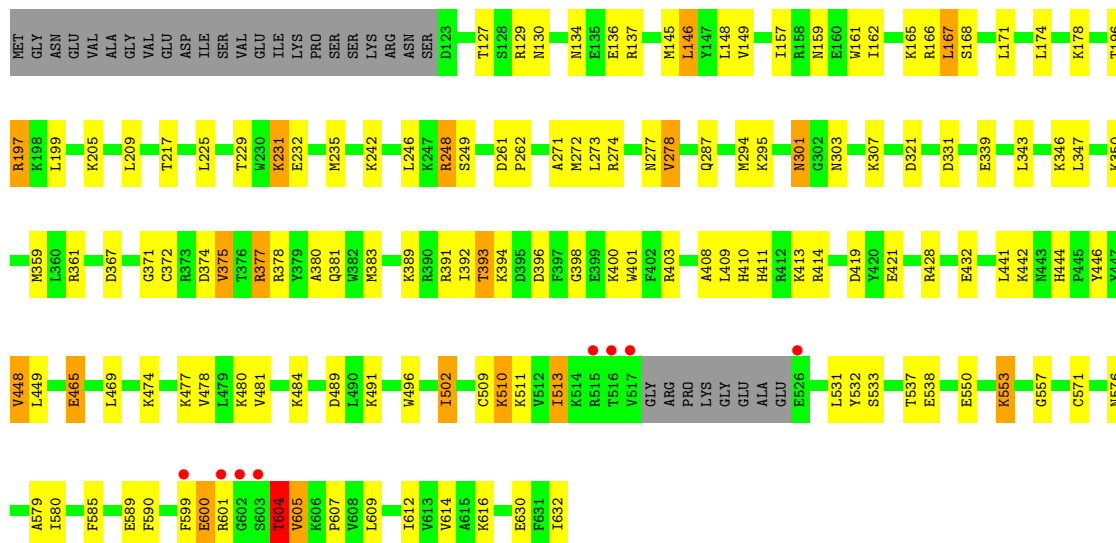
- Molecule 1: native strand of the CPD-mismatch DNA



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

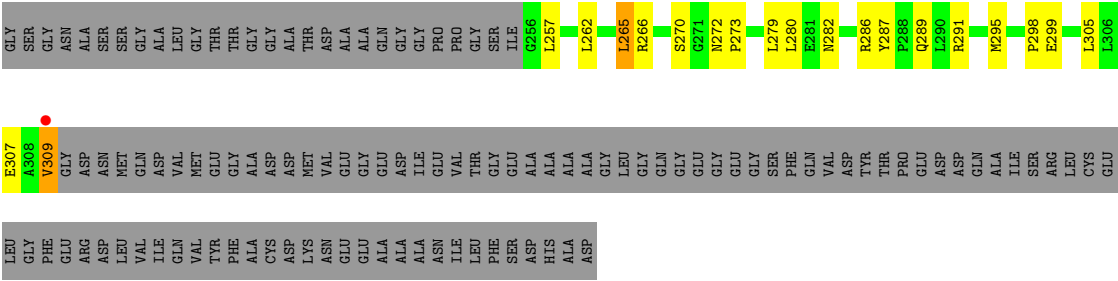


- Molecule 3: DNA repair protein RAD4



- Molecule 4: UV excision repair protein RAD23





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 30.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	93.4 (30.00-3.10) 92.9 (30.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 3.05Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.246 , 0.277 0.264 , 0.255	Depositor DCC
R_{free} test set	1238 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	83.0	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 5.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	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 4.10% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.29	0/537	1.00	1/825 (0.1%)
2	Y	0.27	0/505	0.97	1/778 (0.1%)
3	A	0.45	0/4221	0.80	0/5673
4	X	0.48	0/422	0.90	0/575
All	All	0.42	0/5685	0.85	2/7851 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	13	DG	P-O3'-C3'	5.33	128.19	120.20
1	W	18	DG	P-O3'-C3'	5.11	127.86	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	93	0
4	X	416	0	427	12	0
All	All	5480	0	5169	106	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 (106) 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:H4'	1:W:18:DG:OP1	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:O	3:A:377:ARG:HD3	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:391:ARG:C	3:A:393:THR:H	2.11	0.58
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
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: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
3:A:174:LEU:HB2	3:A:272:MET:HE2	1.92	0.52
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:X:289:GLN:H	4:X:289:GLN:CD	2.21	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:137:ARG:HG2	3:A:294:MET:HE3	1.96	0.48
3:A:287:GLN:HE22	3:A:359:MET:N	2.11	0.48
3:A:600:GLU:HB3	3:A:601:ARG:NE	2.28	0.48
3:A:600:GLU:CB	3:A:601:ARG:NH2	2.77	0.47
3:A:465:GLU:H	3:A:465:GLU:CD	2.22	0.47
3:A:287:GLN:HE22	3:A:359:MET:H	1.61	0.47
3:A:377:ARG:HD3	3:A:377:ARG:C	2.39	0.47
3:A:391:ARG:C	3:A:393:THR:N	2.73	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:174:LEU:CB	3:A:272:MET:HE2	2.45	0.46
3:A:509:CYS:HB2	3:A:531:LEU:O	2.15	0.46
3:A:599:PHE:O	3:A:600:GLU:CB	2.62	0.45
3:A:585:PHE:CD2	3:A:632:ILE:HG23	2.51	0.45
3:A:590:PHE:CD1	3:A:612:ILE:HD12	2.51	0.45
1:W:17:DT:C2	3:A:607:PRO:HG3	2.52	0.45
3:A:287:GLN:NE2	3:A:359:MET:N	2.64	0.45
3:A:205:LYS:O	3:A:209:LEU:HG	2.18	0.44
3:A:301:ASN:HD22	3:A:303:ASN:H	1.65	0.44
3:A:449:LEU:HD23	3:A:481:VAL:HG22	1.99	0.43
4:X:282:ASN:HD21	4:X:286:ARG:HH21	1.65	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:231:LYS:HE2	3:A:235:MET:HE2	2.00	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:157:ILE:HG21	4:X:270:SER:HB2	2.00	0.43
3:A:585:PHE:CG	3:A:632:ILE:HG12	2.54	0.43
3:A:510:LYS:HD3	3:A:533:SER:HB3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:401:TRP:CD1	4:X:298:PRO:HG3	2.54	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:391:ARG:O	3:A:394:LYS:HG2	2.19	0.42
3:A:197:ARG:HD3	3:A:197:ARG:C	2.44	0.42
3:A:389:LYS:O	3:A:394:LYS:HE3	2.20	0.42
2:Y:18:DT:H5'	3:A:137:ARG:HH12	1.84	0.42
3:A:146:LEU:HD22	4:X:280:LEU:HD22	2.02	0.42
3:A:491:LYS:HB2	3:A:496:TRP:CE2	2.55	0.41
3:A:576:ASN:HB3	3:A:579:ALA:HB2	2.02	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:162:ILE:HG23	3:A:271:ALA:HA	2.03	0.41
3:A:225:LEU:HD21	4:X:273:PRO:HG2	2.02	0.41
3:A:377:ARG:HD2	3:A:428:ARG:HB3	2.03	0.41
3:A:553:LYS:HG3	3:A:557:GLY:HA2	2.03	0.41
1:W:19:DC:H2''	1:W:20:DT:OP2	2.21	0.41
3:A:331:ASP:HB2	3:A:347:LEU:HD21	2.03	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:261:ASP:HB2	3:A:262:PRO:CD	2.51	0.40
3:A:513:ILE:HD13	3:A:531:LEU:HD11	2.03	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 [i](#)

5.3.1 Protein backbone [i](#)

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%)	30	63
4	X	52/171 (30%)	46 (88%)	6 (12%)	0	100	100
All	All	550/704 (78%)	506 (92%)	42 (8%)	2 (0%)	30	63

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%)	405 (90%)	47 (10%)	5	22
4	X	47/129 (36%)	40 (85%)	7 (15%)	2	10
All	All	499/606 (82%)	445 (89%)	54 (11%)	5	21

All (54) 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
3	A	148	LEU
3	A	165	LYS
3	A	166	ARG
3	A	167	LEU
3	A	168	SER
3	A	178	LYS
3	A	197	ARG
3	A	199	LEU
3	A	217	THR
3	A	231	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	242	LYS
3	A	248	ARG
3	A	249	SER
3	A	277	ASN
3	A	278	VAL
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	441	LEU
3	A	442	LYS
3	A	448	VAL
3	A	465	GLU
3	A	469	LEU
3	A	478	VAL
3	A	489	ASP
3	A	502	ILE
3	A	510	LYS
3	A	511	LYS
3	A	513	ILE
3	A	553	LYS
3	A	604	THR
3	A	605	VAL
3	A	609	LEU
3	A	614	VAL
3	A	630	GLU
4	X	265	LEU
4	X	279	LEU
4	X	291	ARG
4	X	295	MET
4	X	299	GLU
4	X	307	GLU
4	X	309	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	130	ASN
3	A	134	ASN
3	A	154	HIS
3	A	159	ASN
3	A	173	ASN
3	A	267	GLN
3	A	287	GLN
3	A	301	ASN
3	A	303	ASN
3	A	410	HIS
3	A	411	HIS
3	A	444	HIS
3	A	499	ASN
4	X	267	GLN
4	X	272	ASN
4	X	297	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	W	24/24 (100%)	0.55	2 (8%) 19 10	55, 70, 78, 99	0
2	Y	22/24 (91%)	0.88	3 (13%) 8 5	56, 72, 85, 107	0
3	A	502/533 (94%)	0.11	8 (1%) 70 52	58, 65, 80, 108	0
4	X	54/171 (31%)	-0.09	1 (1%) 66 47	58, 65, 77, 84	0
All	All	602/752 (80%)	0.14	14 (2%) 61 42	55, 66, 81, 108	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	516	THR	4.2
2	Y	11	DT	4.1
4	X	309	VAL	3.8
1	W	24	DA	3.4
3	A	602	GLY	3.4
1	W	1	DT	3.3
3	A	517	VAL	3.1
2	Y	2	DT	3.0
3	A	526	GLU	2.8
3	A	603	SER	2.4
3	A	601	ARG	2.4
2	Y	3	DT	2.1
3	A	515	ARG	2.0
3	A	599	PHE	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 monosaccharides 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.