



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 01:44 pm BST

PDB ID : 5XZW  
Title : Crystal structure of Rad53 1-466  
Authors : Weng, J.H.; Tsai, M.D.  
Deposited on : 2017-07-14  
Resolution : 2.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

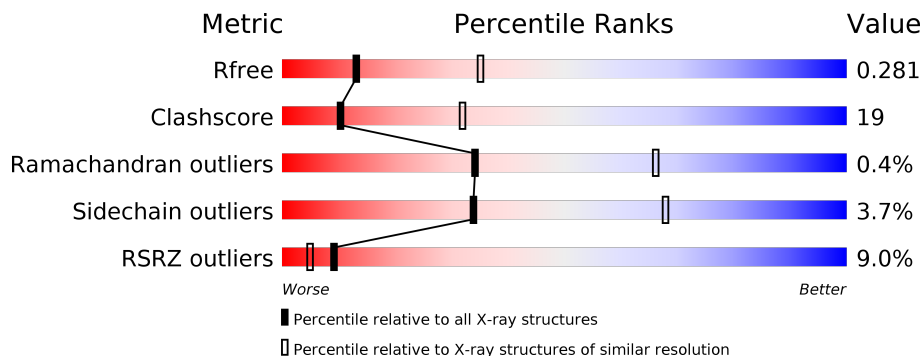
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	471	 10% 50% 28% • 20%
1	B	471	 4% 56% 23% • 20%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5648 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 Serine/threonine-protein kinase RAD53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	378	2693	1698	465	518	12	0	0	0
1	B	379	2906	1849	502	542	13	0	0	0

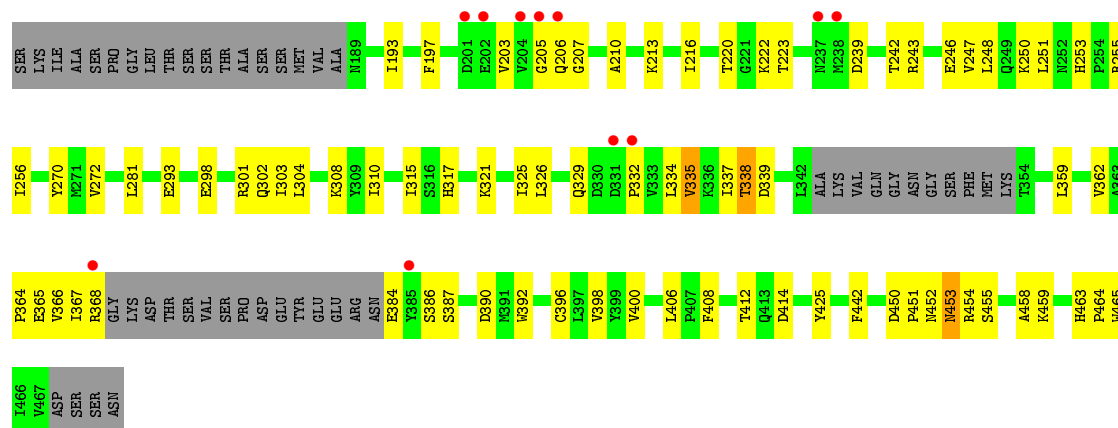
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	467	VAL	-	expression tag	UNP P22216
A	468	ASP	-	expression tag	UNP P22216
A	469	SER	-	expression tag	UNP P22216
A	470	SER	-	expression tag	UNP P22216
A	471	ASN	-	expression tag	UNP P22216
B	467	VAL	-	expression tag	UNP P22216
B	468	ASP	-	expression tag	UNP P22216
B	469	SER	-	expression tag	UNP P22216
B	470	SER	-	expression tag	UNP P22216
B	471	ASN	-	expression tag	UNP P22216

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total 23	O 23	0	0
2	B	26	Total 26	O 26	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.81Å 115.81Å 141.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.53 – 2.80 29.53 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (29.53-2.80) 91.6 (29.53-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.92 (at 2.80Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.267 , 0.284 0.263 , 0.281	Depositor DCC
$R_{free}$ test set	1994 reflections (7.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.9	Xtrriage
Anisotropy	0.031	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 84.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.030 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	5648	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	A	0.43	0/2723	0.63	0/3685
1	B	0.36	0/2954	0.55	0/3992
All	All	0.39	0/5677	0.59	0/7677

There are no bond length outliers.

There are no bond angle outliers.

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	A	2693	0	2499	131	1
1	B	2906	0	2882	80	1
2	A	23	0	0	0	0
2	B	26	0	0	0	0
All	All	5648	0	5381	205	1

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 19.

All (205) 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:A:68:PHE:CD2	1:A:76:TYR:HB3	1.49	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LYS:HB2	1:A:361:TYR:OH	1.17	1.31
1:A:281:LEU:O	1:A:285:VAL:HG13	1.39	1.22
1:A:206:GLN:OE1	1:B:205:GLY:HA2	1.05	1.20
1:A:206:GLN:OE1	1:B:205:GLY:CA	1.94	1.13
1:A:68:PHE:CD2	1:A:76:TYR:CB	2.32	1.11
1:A:68:PHE:HD2	1:A:76:TYR:CB	1.64	1.10
1:A:321:LYS:CB	1:A:361:TYR:OH	2.11	0.98
1:A:28:ILE:HD11	1:A:32:ILE:HG13	1.44	0.97
1:A:281:LEU:O	1:A:285:VAL:CG1	2.16	0.94
1:A:317:HIS:NE2	1:A:339:ASP:O	2.07	0.87
1:A:251:LEU:HD23	1:A:256:ILE:HG21	1.58	0.85
1:A:27:GLN:HA	1:A:27:GLN:HE21	1.40	0.85
1:A:282:MET:O	1:A:285:VAL:HG22	1.75	0.84
1:B:42:GLN:OE1	1:B:42:GLN:N	2.12	0.83
1:A:28:ILE:CD1	1:A:32:ILE:HG13	2.10	0.82
1:A:331:ASP:CB	1:A:332:PRO:HD3	2.10	0.80
1:A:68:PHE:HD2	1:A:76:TYR:HB3	0.73	0.79
1:A:291:VAL:HG21	1:A:401:ILE:HB	1.66	0.77
1:A:321:LYS:HB2	1:A:361:TYR:HH	1.48	0.77
1:A:69:GLY:O	1:A:77:HIS:HA	1.85	0.77
1:A:359:LEU:O	1:A:361:TYR:N	2.19	0.75
1:A:254:PRO:HB2	1:A:255:ARG:NH1	2.03	0.74
1:A:68:PHE:CE2	1:A:76:TYR:CB	2.71	0.73
1:A:276:VAL:HB	1:A:326:LEU:HD23	1.71	0.72
1:B:329:GLN:OE1	1:B:332:PRO:HG2	1.89	0.72
1:A:28:ILE:HD12	1:A:29:GLY:H	1.55	0.71
1:A:56:LEU:HD22	1:A:159:LYS:HB3	1.72	0.71
1:A:317:HIS:CE1	1:A:320:LEU:HD12	2.25	0.71
1:A:27:GLN:HA	1:A:27:GLN:NE2	2.05	0.70
1:A:88:HIS:O	1:A:104:ILE:O	2.09	0.70
1:A:359:LEU:O	1:A:362:VAL:N	2.25	0.70
1:A:282:MET:HB2	1:A:322:PRO:HB2	1.73	0.68
1:A:292:GLY:O	1:A:296:GLY:N	2.27	0.68
1:B:125:SER:HB2	1:B:128:ASP:HB2	1.75	0.67
1:B:37:ILE:HB	1:B:144:VAL:HG12	1.77	0.66
1:A:276:VAL:HG11	1:A:326:LEU:HB3	1.76	0.66
1:A:25:GLN:OE1	1:A:25:GLN:HA	1.95	0.66
1:B:412:THR:HG22	1:B:414:ASP:H	1.61	0.66
1:A:68:PHE:CE2	1:A:76:TYR:HB2	2.31	0.65
1:A:27:GLN:CA	1:A:27:GLN:HE21	2.10	0.65
1:B:308:LYS:HD2	1:B:458:ALA:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:GLU:OE2	1:B:454:ARG:NH2	2.19	0.64
1:A:282:MET:HE3	1:A:285:VAL:HG21	1.78	0.64
1:A:281:LEU:C	1:A:285:VAL:HG13	2.18	0.63
1:B:37:ILE:HG12	1:B:45:ILE:HD12	1.80	0.63
1:A:32:ILE:HD12	1:A:47:ASP:HB3	1.80	0.63
1:A:191:THR:HG22	1:A:192:GLY:H	1.64	0.63
1:A:391:MET:HA	1:A:394:MET:HB3	1.81	0.63
1:A:281:LEU:HA	1:A:327:ILE:HD11	1.80	0.62
1:A:319:ASP:OD1	1:A:321:LYS:HE2	2.00	0.62
1:A:293:GLU:HA	1:A:402:LEU:HD21	1.80	0.62
1:B:152:LYS:O	1:B:156:GLU:HG2	2.00	0.62
1:A:359:LEU:O	1:A:360:ALA:C	2.37	0.62
1:A:28:ILE:HD11	1:A:32:ILE:CG1	2.24	0.62
1:A:148:ASN:OD1	1:A:150:LYS:HG2	2.00	0.62
1:A:307:ILE:HA	1:A:310:ILE:HG12	1.82	0.61
1:B:239:ASP:O	1:B:243:ARG:HG2	2.01	0.61
1:A:298:GLU:O	1:A:302:GLN:HG3	2.01	0.61
1:A:19:LEU:O	1:A:19:LEU:HG	2.02	0.60
1:B:40:THR:OG1	1:B:42:GLN:NE2	2.34	0.60
1:B:207:GLY:N	1:B:210:ALA:O	2.32	0.60
1:A:303:ILE:O	1:A:307:ILE:HG12	2.02	0.58
1:A:203:VAL:HB	1:B:203:VAL:O	2.04	0.57
1:A:87:LYS:CB	1:A:106:THR:HG22	2.35	0.57
1:A:247:VAL:HG13	1:A:315:ILE:HD12	1.87	0.56
1:A:317:HIS:ND1	1:A:320:LEU:CD1	2.68	0.56
1:A:231:LYS:HD3	1:A:269:TYR:CZ	2.41	0.56
1:B:253:HIS:HB3	1:B:256:ILE:HD12	1.85	0.56
1:A:191:THR:HA	1:A:195:LYS:HG2	1.88	0.56
1:A:317:HIS:HB2	1:A:340:PHE:CD2	2.40	0.56
1:A:89:PHE:CZ	1:A:130:ILE:HD13	2.40	0.55
1:A:96:ASP:OD2	1:A:223:THR:HG23	2.05	0.55
1:A:28:ILE:HD12	1:A:29:GLY:N	2.21	0.55
1:A:78:LEU:HG	1:A:141:LEU:HD22	1.87	0.55
1:A:282:MET:HE2	1:A:285:VAL:CG2	2.37	0.55
1:B:412:THR:HG22	1:B:414:ASP:N	2.23	0.54
1:A:362:VAL:HG13	1:A:362:VAL:O	2.07	0.54
1:B:338:THR:HG22	1:B:339:ASP:H	1.71	0.54
1:A:282:MET:CE	1:A:285:VAL:CG2	2.85	0.54
1:B:293:GLU:HG2	1:B:465:TRP:HE1	1.73	0.54
1:A:399:TYR:O	1:A:403:THR:HG22	2.08	0.54
1:A:391:MET:HE1	1:A:456:THR:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LYS:HD3	1:A:66:TRP:CZ2	2.44	0.53
1:B:61:SER:HB3	1:B:220:THR:HG23	1.91	0.53
1:B:51:ASP:OD2	1:B:54:GLN:NE2	2.41	0.53
1:B:100:LEU:HD22	1:B:121:ASN:HB3	1.88	0.53
1:A:292:GLY:O	1:A:295:ALA:HB3	2.09	0.53
1:A:48:LEU:HD11	1:A:68:PHE:HZ	1.73	0.53
1:A:322:PRO:HD3	1:A:397:LEU:HD13	1.91	0.53
1:A:291:VAL:HG21	1:A:401:ILE:CB	2.37	0.53
1:A:56:LEU:HD11	1:A:158:ASN:HB3	1.91	0.53
1:B:239:ASP:HA	1:B:242:THR:HG22	1.90	0.53
1:A:304:LEU:HD23	1:A:307:ILE:HD11	1.90	0.52
1:A:25:GLN:HG2	1:B:129:GLU:OE2	2.09	0.52
1:A:359:LEU:HA	1:A:362:VAL:HB	1.91	0.52
1:A:282:MET:CE	1:A:285:VAL:HG21	2.39	0.52
1:A:55:VAL:HG13	1:A:63:LYS:HD2	1.89	0.52
1:B:91:ILE:HD12	1:B:124:LEU:HD11	1.91	0.52
1:A:394:MET:O	1:A:398:VAL:HG23	2.09	0.52
1:A:399:TYR:C	1:A:403:THR:HG22	2.30	0.52
1:B:329:GLN:HB3	1:B:334:LEU:HB2	1.92	0.52
1:A:215:ALA:O	1:A:224:PHE:N	2.39	0.52
1:A:255:ARG:HD2	1:A:335:VAL:O	2.09	0.52
1:B:384:GLU:HA	1:B:387:SER:HB3	1.92	0.52
1:B:101:LEU:HD13	1:B:130:ILE:HD13	1.93	0.51
1:A:206:GLN:HB3	1:B:206:GLN:O	2.10	0.51
1:A:282:MET:HA	1:A:285:VAL:HG13	1.93	0.51
1:A:27:GLN:CA	1:A:27:GLN:NE2	2.72	0.51
1:A:317:HIS:CE1	1:A:320:LEU:CD1	2.94	0.51
1:B:302:GLN:OE1	1:B:335:VAL:HG23	2.11	0.51
1:B:248:LEU:HA	1:B:251:LEU:HD13	1.93	0.50
1:A:319:ASP:O	1:A:324:ASN:ND2	2.42	0.50
1:B:303:ILE:HG23	1:B:337:ILE:HD11	1.92	0.50
1:B:455:SER:HA	1:B:459:LYS:HE3	1.92	0.50
1:A:317:HIS:CD2	1:A:339:ASP:O	2.63	0.50
1:B:64:LYS:HG2	1:B:66:TRP:CZ2	2.47	0.50
1:B:450:ASP:OD1	1:B:452:ASN:ND2	2.44	0.49
1:A:197:PHE:CZ	1:A:272:VAL:HG11	2.48	0.49
1:A:63:LYS:HB2	1:A:93:LEU:HG	1.95	0.49
1:A:78:LEU:HD23	1:A:134:VAL:HG21	1.95	0.49
1:A:71:ASN:O	1:A:74:CYS:HB2	2.12	0.49
1:B:110:TRP:CH2	1:B:134:VAL:HB	2.48	0.49
1:B:149:ASP:HA	1:B:152:LYS:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:PHE:CZ	1:B:425:TYR:HB3	2.49	0.48
1:B:81:ILE:HB	1:B:84:LEU:HG	1.95	0.48
1:A:318:ARG:O	1:A:319:ASP:CB	2.62	0.48
1:A:31:ASN:OD1	1:A:31:ASN:N	2.47	0.48
1:A:67:THR:HG22	1:A:90:GLN:HG2	1.96	0.48
1:A:21:GLU:HA	1:A:21:GLU:OE1	2.13	0.48
1:B:463:HIS:CG	1:B:464:PRO:HD2	2.49	0.48
1:A:51:ASP:OD2	1:A:53:SER:OG	2.23	0.47
1:A:139:ASP:N	1:A:139:ASP:OD1	2.46	0.47
1:A:359:LEU:C	1:A:361:TYR:N	2.67	0.47
1:A:271:MET:HB3	1:A:273:MET:HE2	1.97	0.47
1:A:217:GLU:O	1:A:221:GLY:N	2.43	0.47
1:B:298:GLU:OE2	1:B:301:ARG:NH2	2.47	0.47
1:B:220:THR:HG22	1:B:222:LYS:HB2	1.97	0.46
1:A:233:LYS:HE3	1:A:233:LYS:HB2	1.82	0.46
1:A:28:ILE:HD11	1:A:32:ILE:HG21	1.96	0.46
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.74	0.46
1:A:282:MET:HA	1:A:285:VAL:CG1	2.46	0.46
1:A:298:GLU:HA	1:A:301:ARG:NH1	2.31	0.46
1:B:255:ARG:HA	1:B:255:ARG:HD3	1.64	0.45
1:A:419:GLN:O	1:A:423:GLY:N	2.49	0.45
1:B:321:LYS:O	1:B:325:ILE:HG12	2.16	0.45
1:B:250:LYS:HD2	1:B:250:LYS:HA	1.83	0.45
1:B:359:LEU:HA	1:B:362:VAL:HG23	1.99	0.45
1:B:325:ILE:HG22	1:B:335:VAL:HG12	1.99	0.44
1:B:364:PRO:HD3	1:B:392:TRP:CE2	2.53	0.44
1:B:398:VAL:HG21	1:B:442:PHE:HE2	1.83	0.44
1:A:156:GLU:HA	1:A:159:LYS:NZ	2.33	0.44
1:A:282:MET:CA	1:A:285:VAL:HG13	2.47	0.44
1:A:72:PRO:O	1:A:73:ALA:C	2.56	0.44
1:B:310:ILE:HD12	1:B:315:ILE:O	2.17	0.44
1:A:101:LEU:HB2	1:A:124:LEU:HD21	1.99	0.44
1:B:304:LEU:HD11	1:B:442:PHE:HZ	1.82	0.44
1:B:396:CYS:O	1:B:400:VAL:HG23	2.17	0.44
1:B:453:ASN:N	1:B:453:ASN:OD1	2.50	0.44
1:B:61:SER:CB	1:B:220:THR:HG23	2.47	0.44
1:A:199:ILE:HD13	1:A:226:VAL:HG11	1.98	0.44
1:B:317:HIS:NE2	1:B:338:THR:O	2.44	0.44
1:B:243:ARG:HA	1:B:246:GLU:HG3	2.00	0.43
1:B:326:LEU:HG	1:B:338:THR:OG1	2.18	0.43
1:A:248:LEU:HD13	1:A:273:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:TYR:CD1	1:A:361:TYR:O	2.71	0.43
1:B:243:ARG:O	1:B:247:VAL:HG23	2.18	0.43
1:B:34:CYS:SG	1:B:145:ILE:HG23	2.58	0.43
1:B:55:VAL:O	1:B:63:LYS:HD2	2.19	0.43
1:A:268:SER:HB2	1:A:270:TYR:CE1	2.54	0.43
1:B:193:ILE:HD12	1:B:270:TYR:HB3	2.01	0.43
1:B:87:LYS:HB3	1:B:104:ILE:HD11	1.99	0.43
1:A:285:VAL:O	1:A:289:GLY:O	2.36	0.43
1:A:38:CYS:SG	1:A:40:THR:HB	2.59	0.43
1:A:219:THR:HG23	1:A:220:THR:HG23	2.00	0.43
1:A:317:HIS:HB2	1:A:340:PHE:CE2	2.54	0.43
1:B:150:LYS:HD2	1:B:150:LYS:HA	1.57	0.43
1:A:271:MET:HB3	1:A:273:MET:CE	2.48	0.42
1:A:193:ILE:HD12	1:A:270:TYR:HB3	2.01	0.42
1:A:15:THR:HG22	1:A:18:PHE:CB	2.50	0.42
1:A:278:GLY:HA3	1:A:327:ILE:O	2.19	0.42
1:B:98:ASN:ND2	1:B:216:ILE:HD12	2.35	0.42
1:B:40:THR:CB	1:B:42:GLN:HE22	2.32	0.42
1:B:366:VAL:O	1:B:368:ARG:N	2.53	0.42
1:A:110:TRP:HB2	1:A:131:THR:HB	2.02	0.41
1:B:110:TRP:CZ3	1:B:134:VAL:HB	2.55	0.41
1:B:197:PHE:CZ	1:B:272:VAL:HG11	2.55	0.41
1:A:361:TYR:HB3	1:A:396:CYS:SG	2.59	0.41
1:A:43:ILE:HD12	1:A:43:ILE:HA	1.80	0.41
1:A:206:GLN:OE1	1:B:205:GLY:C	2.56	0.41
1:B:251:LEU:HD23	1:B:310:ILE:HG22	2.02	0.41
1:B:450:ASP:HA	1:B:451:PRO:HD2	1.90	0.41
1:B:71:ASN:HA	1:B:72:PRO:HD2	1.91	0.41
1:A:194:PHE:O	1:A:195:LYS:HD3	2.21	0.41
1:A:243:ARG:HG2	1:A:343:ALA:CB	2.51	0.41
1:B:334:LEU:HA	1:B:334:LEU:HD23	1.86	0.41
1:B:281:LEU:HD12	1:B:281:LEU:HA	1.88	0.41
1:B:203:VAL:HG22	1:B:213:LYS:HD3	2.03	0.41
1:B:387:SER:O	1:B:390:ASP:HB2	2.21	0.40
1:A:245:LEU:HD11	1:A:262:PHE:CE1	2.56	0.40
1:B:216:ILE:CD1	1:B:223:THR:HG22	2.52	0.40
1:A:56:LEU:CD2	1:A:159:LYS:HB3	2.47	0.40
1:A:253:HIS:CE1	1:A:305:THR:HG22	2.57	0.40
1:B:255:ARG:NH1	1:B:334:LEU:HD22	2.37	0.40
1:B:400:VAL:HG22	1:B:406:LEU:HD23	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:SER:OG	1:B:450:ASP:OD2[4_455]	2.18	0.02

## 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	
1	A	360/471 (76%)	334 (93%)	24 (7%)	2 (1%)	25	56
1	B	371/471 (79%)	348 (94%)	22 (6%)	1 (0%)	41	72
All	All	731/942 (78%)	682 (93%)	46 (6%)	3 (0%)	34	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	ALA
1	B	367	ILE
1	A	333	VAL

### 5.3.2 Protein sidechains [i](#)

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	257/413 (62%)	245 (95%)	12 (5%)	26	59
1	B	310/413 (75%)	301 (97%)	9 (3%)	42	76
All	All	567/826 (69%)	546 (96%)	21 (4%)	34	68

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	27	GLN
1	A	38	CYS
1	A	39	THR
1	A	89	PHE
1	A	99	LEU
1	A	219	THR
1	A	268	SER
1	A	285	VAL
1	A	291	VAL
1	A	358	THR
1	A	402	LEU
1	B	42	GLN
1	B	52	ILE
1	B	80	ASN
1	B	125	SER
1	B	144	VAL
1	B	335	VAL
1	B	338	THR
1	B	386	SER
1	B	453	ASN

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	27	GLN
1	A	88	HIS
1	A	237	ASN
1	B	413	GLN

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	378/471 (80%)	0.56	47 (12%) <b>4</b> <b>2</b>	37, 73, 147, 169	0
1	B	379/471 (80%)	0.24	21 (5%) <b>25</b> <b>16</b>	42, 62, 102, 138	0
All	All	757/942 (80%)	0.40	68 (8%) <b>9</b> <b>5</b>	37, 65, 131, 169	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	332	PRO	8.7
1	B	205	GLY	8.5
1	A	383	ASN	7.4
1	A	331	ASP	6.8
1	A	411	SER	6.7
1	A	454	ARG	5.1
1	A	160	VAL	5.0
1	A	433	PHE	4.9
1	A	439	ALA	4.8
1	B	139	ASP	4.8
1	A	70	ARG	4.7
1	A	26	GLU	4.4
1	B	138	SER	4.3
1	A	107	ASN	4.3
1	A	288	HIS	4.1
1	A	432	ASP	4.0
1	A	69	GLY	4.0
1	B	137	GLU	3.8
1	B	155	LEU	3.7
1	A	438	GLU	3.6
1	A	138	SER	3.5
1	B	332	PRO	3.5
1	A	437	GLU	3.5
1	A	431	LYS	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	161	ASP	3.2
1	B	385	TYR	3.2
1	B	238	MET	3.2
1	A	455	SER	3.1
1	A	434	ARG	3.1
1	A	106	THR	3.1
1	B	331	ASP	3.0
1	B	53	SER	3.0
1	A	429	PRO	3.0
1	B	201	ASP	2.9
1	A	444	ASP	2.8
1	B	136	VAL	2.8
1	A	413	GLN	2.8
1	B	206	GLN	2.8
1	B	52	ILE	2.7
1	A	367	ILE	2.7
1	A	462	ASN	2.6
1	A	417	TYR	2.6
1	A	463	HIS	2.6
1	A	420	ILE	2.5
1	A	366	VAL	2.5
1	A	158	ASN	2.5
1	A	412	THR	2.5
1	A	163	ILE	2.4
1	A	421	GLY	2.4
1	B	368	ARG	2.4
1	B	134	VAL	2.4
1	A	15	THR	2.4
1	A	114	GLN	2.3
1	B	204	VAL	2.3
1	A	24	SER	2.3
1	A	425	TYR	2.3
1	B	95	GLU	2.3
1	B	43	ILE	2.3
1	A	414	ASP	2.2
1	A	436	SER	2.2
1	B	202	GLU	2.2
1	A	113	GLY	2.1
1	A	333	VAL	2.1
1	A	153	GLN	2.1
1	A	357	GLY	2.1
1	B	237	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	330	ASP	2.0
1	A	361	TYR	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.