



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:56 AM UTC

PDB ID : 5XZW / pdb_00005xzw
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

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

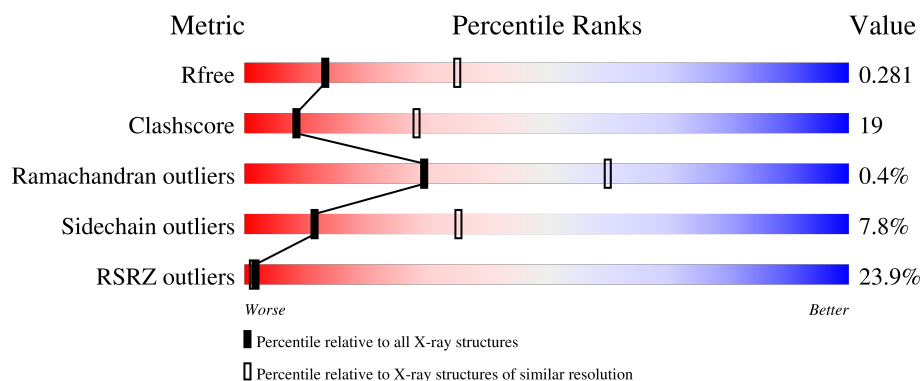
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 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	471	28% 47% 29% • 20%
1	B	471	10% 53% 25% • 20%

2 Entry composition

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.

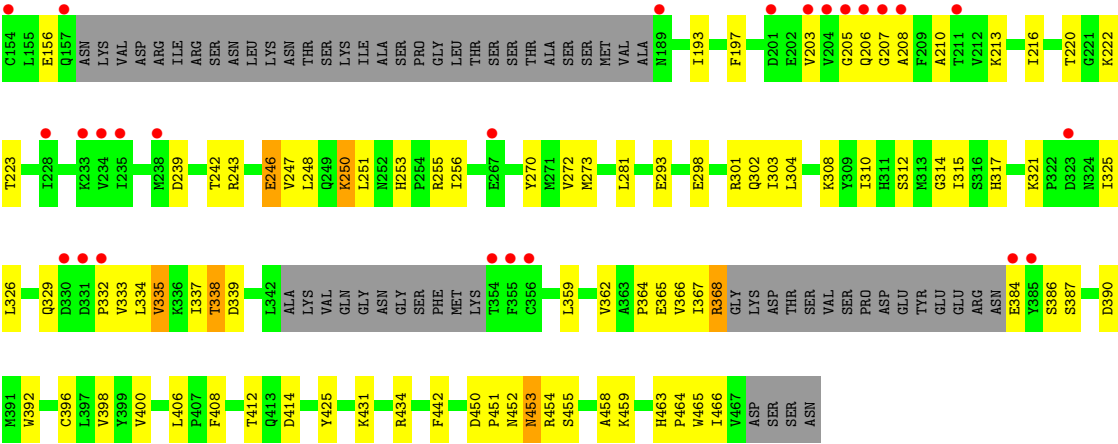
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2693	1698	465	518	12			
1	B	379	Total	C	N	O	S	0	0	0
			2906	1849	502	542	13			

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	O	0	0
			23	23		
2	B	26	Total	O	0	0
			26	26		



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	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) 91.5 (29.53-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.92 (at 2.80Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.267 , 0.284 0.262 , 0.281	Depositor DCC
R_{free} test set	1994 reflections (7.24%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 84.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.030 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5648	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage'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.*

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	0.61	0/2723	1.05	16/3685 (0.4%)
1	B	0.46	0/2954	0.91	6/3992 (0.2%)
All	All	0.54	0/5677	0.98	22/7677 (0.3%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	GLN	N-CA-C	11.60	123.93	111.28
1	A	70	ARG	N-CA-C	8.20	120.22	111.28
1	A	25	GLN	N-CA-C	7.95	119.94	111.28
1	B	57	LYS	N-CA-C	-7.66	104.16	113.97
1	A	163	ILE	N-CA-C	-6.83	105.86	112.29
1	A	338	THR	N-CA-C	6.76	123.15	114.56
1	A	26	GLU	N-CA-C	6.32	123.55	114.39
1	A	71	ASN	N-CA-C	6.19	118.62	110.08
1	B	108	GLY	N-CA-C	6.06	119.63	110.18
1	A	392	TRP	N-CA-C	-5.92	104.74	111.14
1	B	118	LYS	N-CA-C	5.79	118.85	110.28
1	A	450	ASP	CA-C-N	5.75	125.60	119.28
1	A	450	ASP	C-N-CA	5.75	125.60	119.28
1	A	18	PHE	N-CA-C	-5.67	105.10	111.28
1	A	294	ASP	N-CA-C	-5.65	105.12	111.28
1	B	208	ALA	N-CA-C	-5.62	105.16	111.28
1	A	335	VAL	N-CA-C	5.43	116.49	108.45
1	A	237	ASN	N-CA-C	5.38	121.04	113.02
1	B	71	ASN	CA-C-N	5.30	125.02	119.82
1	B	71	ASN	C-N-CA	5.30	125.02	119.82
1	A	462	ASN	N-CA-C	5.17	119.59	113.12
1	A	105	SER	N-CA-C	5.12	118.66	111.90

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	2693	0	2499	131	1
1	B	2906	0	2882	83	1
2	A	23	0	0	0	0
2	B	26	0	0	0	0
All	All	5648	0	5381	207	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 (207) 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
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:282:MET:HE3	1:A:285:VAL:CG2	1.92	0.99
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:282:MET:HE3	1:A:285:VAL:HG21	1.46	0.95
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:HE21	1:A:27:GLN:HA	1.40	0.85
1:A:282:MET:O	1:A:285:VAL:HG22	1.75	0.84
1:B:42:GLN:N	1:B:42:GLN:OE1	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:VAL:HG21	1:A:401:ILE:HB	1.66	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:321:LYS:HB2	1:A:361:TYR:HH	1.53	0.70
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:281:LEU:C	1:A:285:VAL:HG13	2.18	0.68
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:A:359:LEU:O	1:A:360:ALA:C	2.37	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:HE21	1:A:27:GLN:CA	2.10	0.65
1:B:308:LYS:HD2	1:B:458:ALA:HA	1.79	0.64
1:B:365:GLU:OE2	1:B:454:ARG:NH2	2.19	0.64
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:293:GLU:HA	1:A:402:LEU:HD21	1.80	0.62
1:A:319:ASP:OD1	1:A:321:LYS:HE2	2.00	0.62
1:B:152:LYS:O	1:B:156:GLU:HG2	2.00	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:231:LYS:HD3	1:A:269:TYR:CZ	2.41	0.56
1:A:317:HIS:ND1	1:A:320:LEU:CD1	2.68	0.56
1:A:399:TYR:C	1:A:403:THR:HG22	2.30	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: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: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: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:48:LEU:HD11	1:A:68:PHE:HZ	1.73	0.53
1:A:206:GLN:CD	1:B:205:GLY:HA2	2.13	0.53
1:A:292:GLY:O	1:A:295:ALA:HB3	2.09	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:248:LEU:HD13	1:A:273:MET:HE1	1.91	0.52
1:A:359:LEU:HA	1:A:362:VAL:HB	1.91	0.52
1:A:55:VAL:HG13	1:A:63:LYS:HD2	1.89	0.52
1:A:359:LEU:C	1:A:361:TYR:N	2.67	0.52
1:B:91:ILE:HD12	1:B:124:LEU:HD11	1.91	0.52
1:A:391:MET:HE1	1:A:456:THR:HA	1.92	0.52
1:A:394:MET:O	1:A:398:VAL:HG23	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:206:GLN:HB3	1:B:206:GLN:O	2.10	0.51
1:B:101:LEU:HD13	1:B:130:ILE:HD13	1.93	0.51
1:A:282:MET:HA	1:A:285:VAL:HG13	1.93	0.51
1:A:27:GLN:NE2	1:A:27:GLN:CA	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:72:PRO:O	1:A:73:ALA:C	2.56	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
1:B:81:ILE:HB	1:B:84:LEU:HG	1.95	0.48
1:B:408:PHE:CZ	1:B:425:TYR:HB3	2.49	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:OD1	1:A:139:ASP:N	2.46	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:28:ILE:HD11	1:A:32:ILE:HG21	1.96	0.46
1:A:233:LYS:HE3	1:A:233:LYS:HB2	1.82	0.46
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.74	0.46
1:A:206:GLN:OE1	1:B:205:GLY:C	2.56	0.46
1:A:282:MET:HA	1:A:285:VAL:CG1	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLU:HA	1:A:301:ARG:NH1	2.31	0.46
1:B:255:ARG:HD3	1:B:255:ARG:HA	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: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:61:SER:CB	1:B:220:THR:HG23	2.47	0.44
1:B:453:ASN:N	1:B:453:ASN:OD1	2.50	0.44
1:A:391:MET:HE2	1:A:391:MET:HB2	1.78	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:361:TYR:O	1:A:361:TYR:CD1	2.71	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:B:243:ARG:O	1:B:247:VAL:HG23	2.18	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:38:CYS:SG	1:A:40:THR:HB	2.59	0.43
1:A:285:VAL:O	1:A:289:GLY:O	2.36	0.43
1:B:273:MET:HE3	1:B:273:MET:HB3	1.95	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:A:245:LEU:HG	1:A:271:MET:HE2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:251:LEU:HD23	1:B:310:ILE:HG22	2.02	0.41
1:B:71:ASN:HA	1:B:72:PRO:HD2	1.91	0.41
1:B:450:ASP:HA	1:B:451:PRO:HD2	1.90	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:281:LEU:HD12	1:B:281:LEU:HA	1.88	0.41
1:B:334:LEU:HD23	1:B:334:LEU:HA	1.86	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:312:SER:C	1:B:314:GLY:H	2.29	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 symmetry 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

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	360/471 (76%)	334 (93%)	24 (7%)	2 (1%)	21	51
1	B	371/471 (79%)	348 (94%)	22 (6%)	1 (0%)	36	66
All	All	731/942 (78%)	682 (93%)	46 (6%)	3 (0%)	30	60

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 ⓘ

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%)	234 (91%)	23 (9%)	9	29
1	B	310/413 (75%)	289 (93%)	21 (7%)	14	42
All	All	567/826 (69%)	523 (92%)	44 (8%)	11	35

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	27	GLN
1	A	39	THR
1	A	40	THR
1	A	43	ILE
1	A	78	LEU
1	A	89	PHE
1	A	104	ILE
1	A	140	ILE
1	A	163	ILE
1	A	213	LYS
1	A	219	THR
1	A	235	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	259	LEU
1	A	268	SER
1	A	285	VAL
1	A	291	VAL
1	A	305	THR
1	A	307	ILE
1	A	315	ILE
1	A	358	THR
1	A	389	VAL
1	A	402	LEU
1	B	42	GLN
1	B	46	ARG
1	B	52	ILE
1	B	80	ASN
1	B	104	ILE
1	B	106	THR
1	B	125	SER
1	B	136	VAL
1	B	144	VAL
1	B	150	LYS
1	B	246	GLU
1	B	250	LYS
1	B	333	VAL
1	B	335	VAL
1	B	338	THR
1	B	368	ARG
1	B	386	SER
1	B	431	LYS
1	B	434	ARG
1	B	453	ASN
1	B	466	ILE

Sometimes 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 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

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	378/471 (80%)	1.67	134 (35%) 1 0	37, 73, 147, 169	0
1	B	379/471 (80%)	0.94	47 (12%) 8 6	42, 62, 102, 138	0
All	All	757/942 (80%)	1.31	181 (23%) 2 1	37, 65, 131, 169	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	331	ASP	10.0
1	B	205	GLY	7.5
1	A	332	PRO	7.2
1	A	465	TRP	6.8
1	A	462	ASN	6.6
1	A	71	ASN	6.2
1	A	438	GLU	6.2
1	A	70	ARG	6.1
1	A	69	GLY	5.9
1	A	26	GLU	5.8
1	A	294	ASP	5.8
1	A	439	ALA	5.6
1	A	412	THR	5.5
1	A	441	ASP	5.4
1	A	160	VAL	5.4
1	A	424	SER	5.4
1	A	425	TYR	5.2
1	A	357	GLY	5.2
1	A	24	SER	5.1
1	A	455	SER	5.1
1	A	284	PHE	5.0
1	A	361	TYR	4.9
1	A	450	ASP	4.8
1	A	107	ASN	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	41	GLY	4.7
1	A	106	THR	4.7
1	A	138	SER	4.7
1	B	204	VAL	4.6
1	B	125	SER	4.5
1	A	418	LYS	4.5
1	A	411	SER	4.5
1	A	23	PHE	4.4
1	B	157	GLN	4.4
1	A	446	LEU	4.3
1	A	290	ALA	4.3
1	A	17	ARG	4.2
1	A	414	ASP	4.2
1	B	40	THR	4.1
1	B	153	GLN	4.1
1	A	452	ASN	4.1
1	A	461	LEU	4.1
1	B	206	GLN	4.1
1	A	420	ILE	4.0
1	B	234	VAL	4.0
1	B	354	THR	4.0
1	A	288	HIS	3.9
1	B	330	ASP	3.9
1	A	358	THR	3.8
1	B	331	ASP	3.8
1	A	367	ILE	3.8
1	B	207	GLY	3.8
1	A	408	PHE	3.8
1	A	453	ASN	3.7
1	B	108	GLY	3.7
1	A	366	VAL	3.6
1	B	43	ILE	3.6
1	B	139	ASP	3.6
1	A	18	PHE	3.6
1	A	429	PRO	3.6
1	A	330	ASP	3.5
1	B	211	THR	3.5
1	A	390	ASP	3.5
1	A	464	PRO	3.4
1	A	359	LEU	3.4
1	A	430	LEU	3.4
1	B	138	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	297	ARG	3.4
1	A	333	VAL	3.3
1	B	233	LYS	3.3
1	A	305	THR	3.3
1	B	95	GLU	3.3
1	A	72	PRO	3.3
1	A	433	PHE	3.3
1	A	362	VAL	3.3
1	B	136	VAL	3.3
1	A	293	GLU	3.2
1	A	431	LYS	3.2
1	A	108	GLY	3.2
1	B	208	ALA	3.2
1	B	201	ASP	3.1
1	A	393	SER	3.1
1	A	405	HIS	3.1
1	A	68	PHE	3.1
1	A	432	ASP	3.0
1	A	25	GLN	3.0
1	A	42	GLN	3.0
1	A	113	GLY	3.0
1	A	334	LEU	3.0
1	B	137	GLU	3.0
1	A	422	ARG	3.0
1	A	295	ALA	3.0
1	A	22	LYS	3.0
1	A	139	ASP	3.0
1	A	341	GLY	2.9
1	A	407	PRO	2.9
1	A	142	SER	2.9
1	A	110	TRP	2.9
1	A	399	TYR	2.9
1	A	323	ASP	2.9
1	A	392	TRP	2.8
1	A	117	GLU	2.8
1	A	383	ASN	2.8
1	B	189	ASN	2.8
1	B	355	PHE	2.8
1	A	296	GLY	2.8
1	B	384	GLU	2.8
1	A	338	THR	2.8
1	B	39	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	49	SER	2.8
1	A	285	VAL	2.8
1	A	413	GLN	2.7
1	A	77	HIS	2.7
1	A	15	THR	2.7
1	A	40	THR	2.7
1	A	456	THR	2.7
1	B	52	ILE	2.7
1	A	119	ASN	2.7
1	A	89	PHE	2.7
1	B	228	ILE	2.7
1	A	159	LYS	2.6
1	A	442	PHE	2.6
1	A	105	SER	2.6
1	A	434	ARG	2.6
1	A	154	CYS	2.6
1	B	69	GLY	2.6
1	A	74	CYS	2.6
1	A	396	CYS	2.6
1	B	267	GLU	2.6
1	A	463	HIS	2.5
1	A	161	ASP	2.5
1	A	134	VAL	2.5
1	B	203	VAL	2.5
1	A	103	ASP	2.5
1	A	133	GLY	2.5
1	A	435	ILE	2.5
1	B	385	TYR	2.5
1	B	154	CYS	2.5
1	A	238	MET	2.5
1	A	460	ALA	2.5
1	B	41	GLY	2.4
1	A	286	ALA	2.4
1	A	329	GLN	2.4
1	A	402	LEU	2.4
1	A	459	LYS	2.4
1	B	128	ASP	2.4
1	B	53	SER	2.4
1	A	20	ILE	2.4
1	A	140	ILE	2.4
1	A	327	ILE	2.4
1	A	437	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	444	ASP	2.3
1	A	287	ALA	2.3
1	B	133	GLY	2.3
1	A	436	SER	2.3
1	B	323	ASP	2.3
1	B	356	CYS	2.3
1	B	82	SER	2.3
1	A	164	ARG	2.2
1	A	16	GLN	2.2
1	A	419	GLN	2.2
1	A	283	ASP	2.2
1	A	385	TYR	2.2
1	B	235	ILE	2.2
1	A	280	ASP	2.2
1	A	299	ILE	2.2
1	A	157	GLN	2.2
1	A	451	PRO	2.2
1	A	131	THR	2.2
1	A	205	GLY	2.2
1	B	45	ILE	2.1
1	B	238	MET	2.1
1	A	104	ILE	2.1
1	A	389	VAL	2.1
1	B	332	PRO	2.1
1	A	49	SER	2.0
1	A	114	GLN	2.0
1	A	132	VAL	2.0
1	A	454	ARG	2.0
1	B	46	ARG	2.0
1	A	363	ALA	2.0
1	A	291	VAL	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.