



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:27 AM GMT

PDB ID : 2QSF
Title : Crystal structure of the Rad4-Rad23 complex
Authors : Min, J.-H.; Pavletich, N.P.
Deposited on : 2007-07-31
Resolution : 2.35 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

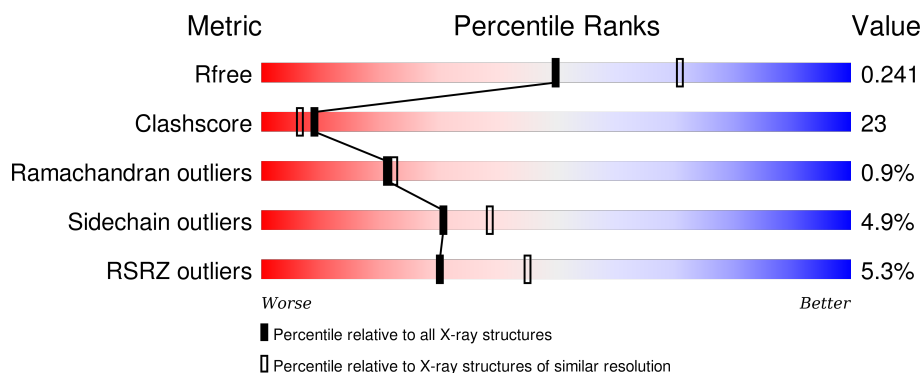
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	533	
2	X	171	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5073 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 DNA repair protein RAD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			4012	2566	720	699	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 2 is a protein called UV excision repair protein RAD23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	104	Total	C	N	O	S	0	0	0
			813	515	132	162	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	228	GLY	-	EXPRESSION TAG	UNP P32628
X	229	SER	-	EXPRESSION TAG	UNP P32628

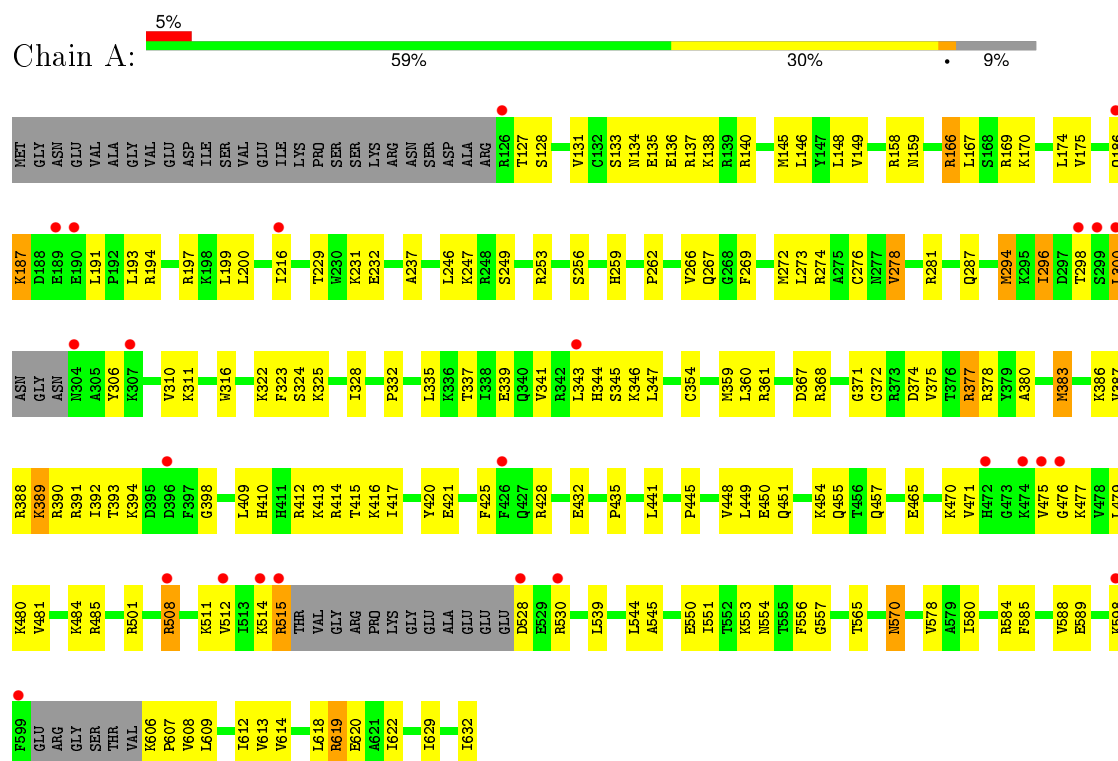
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	220	Total	O	0	0
			220	220		
3	X	28	Total	O	0	0
			28	28		

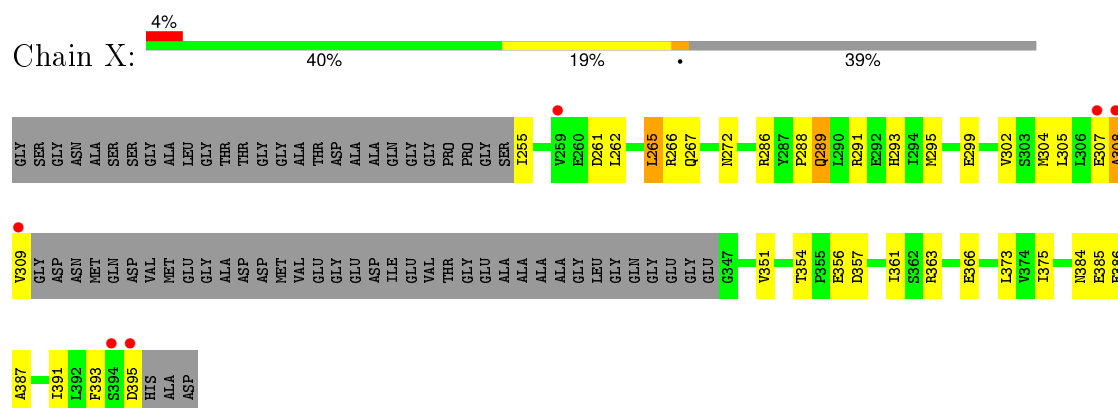
3 Residue-property plots

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: DNA repair protein RAD4



• Molecule 2: UV excision repair protein RAD23



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.17Å 115.71Å 113.95Å 90.00° 105.70° 90.00°	Depositor
Resolution (Å)	15.00 – 2.35 14.96 – 2.34	Depositor EDS
% Data completeness (in resolution range)	90.5 (15.00-2.35) 90.0 (14.96-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.34Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.245 0.208 , 0.241	Depositor DCC
R_{free} test set	1564 reflections (4.01%)	DCC
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 41336 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5073	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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	0.36	0/4099	0.59	0/5505
2	X	0.37	0/825	0.58	0/1120
All	All	0.36	0/4924	0.59	0/6625

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

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	4012	0	4104	190	0
2	X	813	0	794	38	0
3	A	220	0	0	34	0
3	X	28	0	0	2	0
All	All	5073	0	4898	226	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 23.

All (226) 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:508:ARG:HH11	1:A:508:ARG:HB2	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ASP:HA	3:A:662:HOH:O	1.68	0.92
1:A:380:ALA:HB3	1:A:383:MET:HG2	1.52	0.92
1:A:606:LYS:HB2	1:A:607:PRO:HD3	1.57	0.87
1:A:131:VAL:HG23	1:A:294:MET:HB3	1.56	0.86
1:A:306:TYR:HA	3:A:661:HOH:O	1.77	0.84
1:A:159:ASN:HD21	1:A:274:ARG:HH22	1.25	0.84
1:A:170:LYS:HE3	3:A:713:HOH:O	1.78	0.83
1:A:281:ARG:HA	3:A:662:HOH:O	1.77	0.83
1:A:296:ILE:O	1:A:296:ILE:HD13	1.78	0.82
2:X:354:THR:HG22	2:X:356:GLU:H	1.43	0.82
2:X:387:ALA:O	2:X:391:ILE:HG12	1.79	0.82
1:A:580:ILE:H	1:A:580:ILE:HD12	1.46	0.81
1:A:253:ARG:NH1	1:A:253:ARG:HB3	1.96	0.80
1:A:578:VAL:CG1	1:A:629:ILE:HG21	2.11	0.80
1:A:545:ALA:H	1:A:570:ASN:HD21	1.30	0.77
1:A:158:ARG:HH11	1:A:267:GLN:HE22	1.30	0.77
1:A:393:THR:HG23	3:A:655:HOH:O	1.83	0.76
1:A:372:CYS:H	1:A:410:HIS:CD2	2.03	0.76
2:X:386:GLU:H	2:X:386:GLU:CD	1.89	0.75
1:A:508:ARG:HD2	3:A:797:HOH:O	1.86	0.75
1:A:377:ARG:O	1:A:377:ARG:HD3	1.87	0.75
1:A:372:CYS:H	1:A:410:HIS:HD2	1.32	0.75
2:X:363:ARG:O	2:X:366:GLU:HG2	1.86	0.74
1:A:390:ARG:HG3	1:A:390:ARG:HH11	1.50	0.74
2:X:384:ASN:HD21	2:X:386:GLU:HG2	1.54	0.73
2:X:384:ASN:HD22	2:X:387:ALA:CB	2.02	0.71
1:A:565:THR:HG22	3:A:633:HOH:O	1.91	0.70
1:A:578:VAL:HG11	1:A:629:ILE:HG21	1.71	0.70
1:A:375:VAL:HG23	1:A:425:PHE:HZ	1.57	0.69
1:A:391:ARG:HH11	1:A:393:THR:HG21	1.58	0.69
1:A:391:ARG:HB3	1:A:393:THR:HG22	1.76	0.68
1:A:389:LYS:HD3	1:A:390:ARG:HG2	1.74	0.68
1:A:200:LEU:HD21	1:A:328:ILE:HD13	1.75	0.68
1:A:375:VAL:HG21	1:A:378:ARG:NH1	2.07	0.68
2:X:384:ASN:HD22	2:X:387:ALA:H	1.42	0.67
1:A:570:ASN:HD22	1:A:570:ASN:H	1.42	0.67
1:A:377:ARG:HA	1:A:383:MET:HG3	1.77	0.67
1:A:451:GLN:HE22	1:A:479:LEU:HD13	1.59	0.67
1:A:380:ALA:HB1	1:A:387:VAL:HG21	1.77	0.66
1:A:343:LEU:HD12	1:A:344:HIS:N	2.10	0.66
2:X:267:GLN:HE21	2:X:272:ASN:HD22	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LYS:HD2	1:A:420:TYR:CE1	2.31	0.66
1:A:539:LEU:HD11	1:A:565:THR:HG21	1.77	0.65
1:A:614:VAL:HG11	1:A:622:ILE:CD1	2.26	0.65
1:A:606:LYS:HB3	1:A:606:LYS:NZ	2.11	0.65
1:A:137:ARG:HG3	1:A:294:MET:SD	2.36	0.65
2:X:384:ASN:ND2	2:X:387:ALA:H	1.96	0.64
1:A:246:LEU:H	2:X:272:ASN:HD21	1.45	0.64
2:X:354:THR:HG22	2:X:356:GLU:N	2.11	0.64
1:A:391:ARG:CB	1:A:393:THR:HG22	2.28	0.63
1:A:415:THR:HG22	1:A:416:LYS:N	2.14	0.63
1:A:375:VAL:CG2	1:A:378:ARG:NH1	2.62	0.63
1:A:448:VAL:HG22	1:A:484:LYS:HE3	1.81	0.63
1:A:390:ARG:HG3	1:A:390:ARG:NH1	2.08	0.63
1:A:391:ARG:HD3	1:A:393:THR:CG2	2.29	0.62
1:A:580:ILE:N	1:A:580:ILE:HD12	2.14	0.62
1:A:253:ARG:HB3	1:A:253:ARG:HH11	1.61	0.62
1:A:588:VAL:HG22	1:A:589:GLU:H	1.62	0.62
1:A:274:ARG:HD3	1:A:368:ARG:HG2	1.82	0.62
1:A:530:ARG:HD3	3:A:727:HOH:O	1.98	0.62
1:A:159:ASN:ND2	1:A:274:ARG:HH22	1.95	0.62
2:X:267:GLN:HE21	2:X:272:ASN:ND2	1.98	0.62
1:A:345:SER:HB3	3:A:673:HOH:O	1.99	0.61
1:A:298:THR:HG21	3:A:654:HOH:O	2.00	0.61
2:X:363:ARG:HD2	2:X:385:GLU:OE1	2.01	0.61
1:A:322:LYS:HG3	1:A:323:PHE:N	2.15	0.61
1:A:375:VAL:HB	3:A:803:HOH:O	2.00	0.61
1:A:249:SER:O	1:A:253:ARG:HG3	2.00	0.61
1:A:287:GLN:NE2	1:A:361:ARG:HH21	1.99	0.60
1:A:421:GLU:HA	3:A:795:HOH:O	2.02	0.59
1:A:187:LYS:HE3	1:A:187:LYS:HA	1.85	0.59
2:X:255:ILE:HG12	2:X:293:HIS:ND1	2.17	0.59
1:A:128:SER:O	1:A:131:VAL:HG12	2.04	0.58
1:A:166:ARG:HG3	3:A:776:HOH:O	2.03	0.58
2:X:289:GLN:CD	2:X:289:GLN:H	2.06	0.58
1:A:619:ARG:HG3	1:A:619:ARG:HH11	1.68	0.58
1:A:372:CYS:HA	3:A:703:HOH:O	2.02	0.58
1:A:247:LYS:HE2	3:A:838:HOH:O	2.04	0.58
1:A:175:VAL:HG21	1:A:276:CYS:SG	2.43	0.58
1:A:514:LYS:HG2	1:A:515:ARG:N	2.18	0.58
1:A:377:ARG:C	1:A:377:ARG:HD3	2.22	0.57
1:A:415:THR:HG22	1:A:417:ILE:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LYS:HD2	1:A:420:TYR:HE1	1.69	0.57
1:A:465:GLU:CG	1:A:480:LYS:HD2	2.34	0.57
1:A:296:ILE:HG22	3:A:675:HOH:O	2.04	0.57
1:A:570:ASN:H	1:A:570:ASN:ND2	2.02	0.56
2:X:288:PRO:HD2	2:X:289:GLN:NE2	2.20	0.56
2:X:289:GLN:NE2	2:X:289:GLN:H	2.03	0.56
1:A:450:GLU:OE1	1:A:480:LYS:HE3	2.05	0.56
1:A:372:CYS:N	1:A:410:HIS:HD2	2.03	0.56
1:A:377:ARG:NH2	1:A:432:GLU:OE2	2.37	0.56
2:X:391:ILE:O	2:X:395:ASP:HB2	2.05	0.56
1:A:159:ASN:HD21	1:A:274:ARG:NH2	2.00	0.56
1:A:391:ARG:HD3	1:A:393:THR:HG22	1.86	0.56
1:A:588:VAL:HG22	1:A:589:GLU:N	2.21	0.56
1:A:511:LYS:HG2	1:A:512:VAL:N	2.21	0.56
1:A:174:LEU:HB2	1:A:272:MET:HE2	1.87	0.56
1:A:386:LYS:HB3	3:A:851:HOH:O	2.05	0.55
1:A:375:VAL:HG22	1:A:375:VAL:O	2.07	0.55
1:A:310:VAL:HG12	1:A:310:VAL:O	2.07	0.54
2:X:384:ASN:HD22	2:X:387:ALA:HB2	1.72	0.54
1:A:448:VAL:CG2	1:A:484:LYS:HG2	2.38	0.54
1:A:580:ILE:H	1:A:580:ILE:CD1	2.20	0.54
1:A:158:ARG:NH1	1:A:267:GLN:HE22	2.04	0.54
1:A:262:PRO:O	1:A:266:VAL:HG23	2.08	0.53
1:A:570:ASN:HD22	1:A:570:ASN:N	2.01	0.53
1:A:229:THR:HG21	1:A:300:LEU:HD11	1.90	0.53
1:A:158:ARG:HH11	1:A:267:GLN:NE2	2.03	0.53
1:A:514:LYS:HG3	1:A:528:ASP:OD2	2.09	0.53
1:A:588:VAL:HG21	1:A:618:LEU:HD22	1.91	0.53
1:A:413:LYS:HE3	1:A:413:LYS:HA	1.90	0.53
1:A:377:ARG:NH2	3:A:704:HOH:O	2.42	0.53
1:A:266:VAL:HG11	1:A:316:TRP:HA	1.90	0.53
1:A:485:ARG:HG2	1:A:485:ARG:O	2.08	0.52
1:A:166:ARG:HA	1:A:169:ARG:NH1	2.24	0.52
2:X:384:ASN:ND2	2:X:386:GLU:HG2	2.23	0.52
1:A:273:LEU:HB3	1:A:278:VAL:HG22	1.91	0.52
1:A:375:VAL:HG21	1:A:378:ARG:HH12	1.74	0.52
1:A:584:ARG:HG2	1:A:584:ARG:HH11	1.74	0.52
1:A:508:ARG:NH1	1:A:508:ARG:HB2	2.14	0.51
1:A:200:LEU:CD2	1:A:328:ILE:HD13	2.39	0.51
1:A:614:VAL:HG11	1:A:622:ILE:HD12	1.93	0.51
2:X:266:ARG:HG3	2:X:266:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ARG:NH1	3:A:704:HOH:O	2.44	0.51
1:A:359:MET:HE3	3:A:837:HOH:O	2.11	0.51
1:A:435:PRO:HG2	1:A:441:LEU:HG	1.92	0.50
2:X:291:ARG:O	2:X:295:MET:HG2	2.11	0.50
1:A:135:GLU:HG3	3:A:731:HOH:O	2.09	0.50
1:A:325:LYS:HB3	1:A:420:TYR:CD2	2.46	0.50
1:A:585:PHE:CD2	1:A:632:ILE:HG23	2.47	0.50
1:A:127:THR:HG23	3:A:836:HOH:O	2.10	0.50
1:A:347:LEU:N	1:A:347:LEU:HD12	2.26	0.50
1:A:415:THR:CG2	1:A:416:LYS:N	2.75	0.50
1:A:324:SER:HB3	3:A:779:HOH:O	2.11	0.50
1:A:337:THR:HB	3:A:728:HOH:O	2.11	0.49
1:A:528:ASP:N	3:A:801:HOH:O	2.45	0.49
1:A:191:LEU:HD23	1:A:194:ARG:NH1	2.27	0.49
1:A:237:ALA:HB3	3:A:716:HOH:O	2.12	0.49
1:A:281:ARG:NH1	3:A:803:HOH:O	2.45	0.49
1:A:371:GLY:HA2	1:A:410:HIS:HD2	1.78	0.49
1:A:127:THR:OG1	1:A:131:VAL:HG11	2.13	0.49
1:A:578:VAL:HG13	1:A:629:ILE:HG21	1.91	0.48
1:A:371:GLY:HA2	1:A:410:HIS:CD2	2.48	0.48
2:X:391:ILE:HA	2:X:395:ASP:HB2	1.95	0.48
1:A:454:LYS:HB2	1:A:457:GLN:OE1	2.13	0.48
1:A:612:ILE:CD1	1:A:622:ILE:HD13	2.44	0.48
2:X:255:ILE:HD12	2:X:304:MET:CE	2.45	0.47
1:A:448:VAL:CG2	1:A:484:LYS:HE3	2.43	0.47
1:A:550:GLU:HA	1:A:589:GLU:HG2	1.95	0.47
1:A:169:ARG:HD2	3:A:642:HOH:O	2.14	0.47
1:A:528:ASP:N	3:A:743:HOH:O	2.48	0.47
2:X:291:ARG:HD2	3:X:241:HOH:O	2.13	0.47
1:A:606:LYS:HZ3	1:A:606:LYS:HB3	1.79	0.47
2:X:307:GLU:O	2:X:309:VAL:N	2.47	0.47
2:X:384:ASN:ND2	2:X:387:ALA:HB2	2.30	0.47
1:A:380:ALA:CB	1:A:387:VAL:HG21	2.44	0.46
2:X:384:ASN:HD22	2:X:387:ALA:N	2.10	0.46
1:A:253:ARG:HH11	1:A:253:ARG:CB	2.26	0.46
1:A:450:GLU:OE1	1:A:480:LYS:CE	2.63	0.46
1:A:273:LEU:HB3	1:A:278:VAL:CG2	2.46	0.46
1:A:136:GLU:O	1:A:140:ARG:HG3	2.16	0.46
1:A:360:LEU:C	1:A:360:LEU:HD23	2.36	0.45
1:A:619:ARG:NH1	1:A:619:ARG:HG3	2.30	0.45
1:A:598:LYS:O	1:A:606:LYS:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:GLU:HG2	1:A:480:LYS:HD2	1.98	0.45
1:A:300:LEU:N	1:A:300:LEU:HD12	2.31	0.45
1:A:609:LEU:HD12	1:A:609:LEU:N	2.31	0.45
1:A:231:LYS:HE3	1:A:231:LYS:HA	1.98	0.45
1:A:137:ARG:NH1	1:A:137:ARG:HB3	2.32	0.45
1:A:612:ILE:HD12	1:A:614:VAL:HG13	1.98	0.45
1:A:514:LYS:HG2	1:A:515:ARG:H	1.79	0.45
1:A:311:LYS:HD2	1:A:354:CYS:SG	2.57	0.45
1:A:145:MET:O	1:A:149:VAL:HG23	2.17	0.44
2:X:286:ARG:HD2	3:X:223:HOH:O	2.16	0.44
2:X:354:THR:HB	2:X:357:ASP:OD2	2.17	0.44
1:A:554:ASN:OD1	1:A:556:PHE:N	2.51	0.44
1:A:191:LEU:HG	1:A:193:LEU:HB3	2.00	0.44
1:A:412:ARG:HH11	1:A:412:ARG:HG3	1.83	0.44
1:A:620:GLU:OE1	1:A:620:GLU:HA	2.18	0.44
1:A:454:LYS:HE3	1:A:455:GLN:H	1.82	0.44
1:A:374:ASP:OD1	1:A:391:ARG:NH2	2.46	0.44
1:A:612:ILE:HD11	1:A:622:ILE:HD13	1.99	0.44
1:A:339:GLU:OE1	1:A:346:LYS:HG3	2.17	0.44
1:A:166:ARG:HH12	1:A:256:SER:HB3	1.83	0.44
1:A:514:LYS:CG	1:A:515:ARG:N	2.81	0.43
1:A:391:ARG:HD3	1:A:393:THR:HG21	2.01	0.43
1:A:413:LYS:HE3	3:A:667:HOH:O	2.17	0.43
1:A:377:ARG:HD2	1:A:428:ARG:HB2	2.01	0.43
1:A:134:ASN:O	1:A:138:LYS:HG3	2.18	0.43
2:X:354:THR:CG2	2:X:356:GLU:HB3	2.48	0.43
1:A:539:LEU:CD1	1:A:565:THR:HG21	2.45	0.43
1:A:229:THR:OG1	1:A:232:GLU:HG3	2.19	0.43
2:X:384:ASN:HB3	2:X:387:ALA:HB3	2.01	0.42
2:X:261:ASP:CG	2:X:286:ARG:HH22	2.22	0.42
1:A:471:VAL:O	1:A:476:GLY:HA3	2.19	0.42
1:A:392:ILE:O	1:A:398:GLY:HA3	2.19	0.42
1:A:609:LEU:N	1:A:609:LEU:CD1	2.82	0.42
1:A:186:GLN:OE1	1:A:186:GLN:N	2.52	0.42
1:A:339:GLU:OE2	1:A:341:VAL:HG22	2.19	0.42
1:A:580:ILE:HB	3:A:785:HOH:O	2.19	0.42
1:A:229:THR:CG2	1:A:300:LEU:HD11	2.50	0.42
2:X:307:GLU:O	2:X:308:ALA:C	2.57	0.42
2:X:265:LEU:HD22	2:X:305:LEU:HD21	2.02	0.41
1:A:269:PHE:CG	1:A:332:PRO:HG3	2.55	0.41
1:A:368:ARG:HG3	3:A:638:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LYS:O	1:A:394:LYS:HD3	2.19	0.41
1:A:471:VAL:HG23	1:A:477:LYS:O	2.20	0.41
1:A:511:LYS:CG	1:A:512:VAL:N	2.82	0.41
1:A:470:LYS:HG3	3:A:749:HOH:O	2.21	0.41
1:A:137:ARG:HB3	1:A:137:ARG:HH11	1.86	0.41
1:A:375:VAL:CG2	1:A:378:ARG:HH12	2.32	0.41
1:A:377:ARG:HB2	3:A:679:HOH:O	2.20	0.41
2:X:354:THR:HG22	2:X:356:GLU:HB3	2.02	0.41
1:A:253:ARG:HB3	1:A:253:ARG:CZ	2.50	0.41
1:A:335:LEU:HD12	1:A:347:LEU:HG	2.03	0.41
2:X:361:ILE:HD13	2:X:375:ILE:HG12	2.02	0.41
1:A:409:LEU:CD1	2:X:302:VAL:HG11	2.51	0.41
1:A:136:GLU:HA	1:A:136:GLU:OE2	2.21	0.41
1:A:598:LYS:HG2	1:A:608:VAL:CG2	2.52	0.40
1:A:553:LYS:HD2	1:A:557:GLY:O	2.21	0.40
1:A:388:ARG:HD3	1:A:445:PRO:HD3	2.03	0.40
1:A:551:ILE:HD13	1:A:613:VAL:HG12	2.04	0.40
1:A:174:LEU:CB	1:A:272:MET:HE2	2.52	0.40
1:A:216:ILE:HB	1:A:259:HIS:CD2	2.57	0.40
1:A:449:LEU:HD23	1:A:481:VAL:HG22	2.03	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	
1	A	478/533 (90%)	454 (95%)	21 (4%)	3 (1%)	30	34
2	X	100/171 (58%)	95 (95%)	3 (3%)	2 (2%)	9	6
All	All	578/704 (82%)	549 (95%)	24 (4%)	5 (1%)	21	22

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	X	308	ALA
2	X	393	PHE
1	A	414	ARG
1	A	133	SER
1	A	475	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	439/477 (92%)	419 (95%)	20 (5%)	33	42
2	X	90/129 (70%)	84 (93%)	6 (7%)	20	22
All	All	529/606 (87%)	503 (95%)	26 (5%)	31	39

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	LEU
1	A	148	LEU
1	A	166	ARG
1	A	167	LEU
1	A	187	LYS
1	A	197	ARG
1	A	199	LEU
1	A	278	VAL
1	A	294	MET
1	A	296	ILE
1	A	300	LEU
1	A	377	ARG
1	A	383	MET
1	A	389	LYS
1	A	501	ARG
1	A	508	ARG
1	A	515	ARG
1	A	544	LEU
1	A	570	ASN

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Mol	Chain	Res	Type
1	A	619	ARG
2	X	262	LEU
2	X	265	LEU
2	X	289	GLN
2	X	299	GLU
2	X	351	VAL
2	X	373	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	HIS
1	A	159	ASN
1	A	259	HIS
1	A	267	GLN
1	A	287	GLN
1	A	340	GLN
1	A	410	HIS
1	A	427	GLN
1	A	451	GLN
1	A	455	GLN
1	A	472	HIS
1	A	499	ASN
1	A	570	ASN
2	X	272	ASN
2	X	282	ASN
2	X	289	GLN
2	X	359	GLN
2	X	384	ASN
2	X	390	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 [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	486/533 (91%)	0.22	25 (5%) 32 46	23, 53, 91, 120	0
2	X	104/171 (60%)	0.23	6 (5%) 26 40	32, 56, 89, 119	0
All	All	590/704 (83%)	0.22	31 (5%) 30 45	23, 53, 91, 120	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	599	PHE	7.8
1	A	515	ARG	6.6
1	A	298	THR	6.5
2	X	395	ASP	6.1
1	A	190	GLU	5.5
1	A	304	ASN	5.4
1	A	189	GLU	5.1
2	X	309	VAL	4.4
2	X	394	SER	4.1
1	A	300	LEU	3.9
1	A	475	VAL	3.8
1	A	476	GLY	3.6
1	A	508	ARG	3.4
1	A	216	ILE	3.4
1	A	598	LYS	3.3
2	X	308	ALA	3.2
2	X	259	VAL	3.2
1	A	472	HIS	3.1
1	A	299	SER	2.9
1	A	126	ARG	2.7
1	A	530	ARG	2.7
1	A	474	LYS	2.6
1	A	396	ASP	2.5
2	X	307	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	343	LEU	2.4
1	A	514	LYS	2.3
1	A	307	LYS	2.3
1	A	186	GLN	2.1
1	A	426	PHE	2.1
1	A	528	ASP	2.0
1	A	512	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 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.