



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2016 – 08:31 PM EST

PDB ID : 1D9X  
Title : CRYSTAL STRUCTURE OF THE DNA REPAIR PROTEIN UVRB  
Authors : Theis, K.; Chen, P.J.; Skorvaga, M.; Van Houten, B.; Kisker, C.  
Deposited on : 1999-10-30  
Resolution : 2.60 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

<http://wwpdb.org/validation/2016/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  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

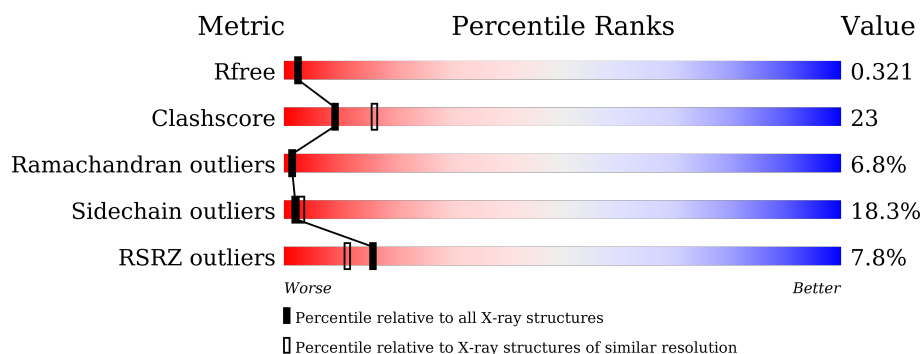
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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	658	<div> <div>7%</div> <div>44%</div> <div>33%</div> <div>11%</div> <div>• 10%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4717 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 EXCINUCLEASE UVRABC COMPONENT UVRB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	0	0
			4632	2916	826	879	11			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total	O	0	0
			83	83		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.21 Å   150.21 Å   79.52 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.60) 100.0 (19.84-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.59 Å)	Xtriage
Refinement program	REFMAC, XPLOR	Depositor
R, $R_{free}$	0.256 , 0.324 0.255 , 0.321	Depositor DCC
$R_{free}$ test set	1632 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.4	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4717	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.77	0/4705	1.48	52/6365 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	ARG	NE-CZ-NH2	-15.97	112.31	120.30
1	A	298	ARG	NE-CZ-NH2	-13.52	113.54	120.30
1	A	447	ARG	NE-CZ-NH1	12.93	126.77	120.30
1	A	447	ARG	CD-NE-CZ	12.72	141.41	123.60
1	A	270	ARG	NE-CZ-NH2	-11.63	114.49	120.30
1	A	413	ARG	CD-NE-CZ	10.60	138.44	123.60
1	A	206	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	A	441	ARG	NH1-CZ-NH2	8.83	129.11	119.40
1	A	252	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	A	257	ARG	NE-CZ-NH2	8.59	124.59	120.30
1	A	289	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	A	316	ARG	NE-CZ-NH2	-8.49	116.05	120.30
1	A	206	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	A	348	ARG	CD-NE-CZ	8.05	134.87	123.60
1	A	289	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	252	ARG	NE-CZ-NH2	-7.57	116.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	523	ASP	CB-CG-OD1	-7.49	111.56	118.30
1	A	300	MET	CA-CB-CG	7.36	125.81	113.30
1	A	289	ARG	CD-NE-CZ	7.31	133.84	123.60
1	A	569	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	A	203	PRO	N-CA-CB	6.83	111.50	103.30
1	A	30	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	A	570	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	270	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	275	ARG	CD-NE-CZ	6.03	132.04	123.60
1	A	474	TYR	CG-CD1-CE1	6.02	126.11	121.30
1	A	311	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	174	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	552	TYR	CB-CG-CD1	5.91	124.54	121.00
1	A	123	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	291	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	A	586	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	A	116	ASN	C-N-CA	5.65	135.81	121.70
1	A	351	TYR	CB-CG-CD2	5.57	124.34	121.00
1	A	351	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	A	529	ARG	CD-NE-CZ	-5.50	115.91	123.60
1	A	444	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	281	LEU	C-N-CA	5.44	135.30	121.70
1	A	552	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	A	569	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	A	425	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	543	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	298	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	355	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	540	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	298	ARG	CD-NE-CZ	-5.12	116.43	123.60
1	A	520	LEU	N-CA-C	5.11	124.80	111.00
1	A	554	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	A	209	HIS	C-N-CA	5.07	134.37	121.70
1	A	127	THR	CA-CB-OG1	5.07	119.64	109.00
1	A	11	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	A	532	ARG	CD-NE-CZ	5.01	130.61	123.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	225	ALA	Mainchain
1	A	268	GLU	Mainchain

## 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	4632	0	4577	212	0
2	A	2	0	0	0	0
3	A	83	0	0	6	0
All	All	4717	0	4577	212	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 (212) 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:493:LEU:HG	1:A:592:ILE:HD13	1.49	0.93
1:A:274:LEU:HB3	1:A:283:ALA:HB1	1.48	0.92
1:A:60:THR:HG22	1:A:334:LEU:HB3	1.54	0.88
1:A:284:GLN:O	1:A:285:ARG:HB3	1.77	0.83
1:A:252:ARG:HD2	1:A:255:LYS:HE2	1.60	0.83
1:A:14:GLN:H	1:A:17:GLN:HE21	1.28	0.81
1:A:168:GLU:HB3	1:A:171:ALA:H	1.46	0.80
1:A:286:LEU:HB3	1:A:365:GLY:O	1.82	0.79
1:A:459:GLU:HG3	1:A:475:LEU:HG	1.64	0.78
1:A:274:LEU:HB3	1:A:283:ALA:CB	2.15	0.76
1:A:148:LEU:HD23	1:A:328:TYR:CE1	2.20	0.76
1:A:289:ARG:HH22	1:A:366:PHE:HB3	1.52	0.74
1:A:375:ARG:HB2	1:A:376:PRO:HD2	1.70	0.73
1:A:85:ALA:HB1	1:A:136:VAL:HG13	1.69	0.73
1:A:479:ILE:HD13	1:A:484:ARG:HG2	1.70	0.71
1:A:473:ALA:HB3	1:A:499:LEU:HA	1.71	0.70
1:A:578:ASN:HA	1:A:583:ILE:HD12	1.72	0.70
1:A:274:LEU:HD22	1:A:283:ALA:HA	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HD13	1:A:290:THR:HG21	1.75	0.69
1:A:455:LYS:O	1:A:475:LEU:HD21	1.93	0.68
1:A:479:ILE:H	1:A:479:ILE:HD12	1.58	0.68
1:A:476:HIS:NE2	1:A:478:GLU:HG3	2.10	0.66
1:A:474:TYR:HD1	1:A:475:LEU:N	1.94	0.65
1:A:200:GLU:O	1:A:219:GLU:HA	1.96	0.65
1:A:503:ASN:O	1:A:506:ARG:HG3	1.96	0.65
1:A:90:VAL:HG22	1:A:91:SER:H	1.60	0.65
1:A:162:ARG:HH11	1:A:240:HIS:HB2	1.61	0.65
1:A:49:ILE:CG2	1:A:336:ILE:HD13	2.27	0.64
1:A:101:TYR:HD1	1:A:108:TYR:HA	1.62	0.64
1:A:168:GLU:HB3	1:A:171:ALA:N	2.12	0.64
1:A:284:GLN:O	1:A:285:ARG:CB	2.45	0.64
1:A:73:LEU:O	1:A:77:LEU:HB2	1.97	0.64
1:A:475:LEU:O	1:A:475:LEU:HD22	1.98	0.63
1:A:239:GLU:CD	1:A:239:GLU:H	2.01	0.63
1:A:286:LEU:HD23	1:A:286:LEU:H	1.63	0.62
1:A:87:GLU:HG3	1:A:126:ALA:HA	1.80	0.62
1:A:348:ARG:NH1	3:A:710:HOH:O	2.32	0.62
1:A:471:LYS:HB3	1:A:496:TYR:HA	1.81	0.62
1:A:278:GLY:HA3	3:A:722:HOH:O	2.01	0.61
1:A:271:LEU:HD21	1:A:286:LEU:HD21	1.83	0.61
1:A:411:ILE:HD11	1:A:573:ILE:HG21	1.83	0.60
1:A:335:ILE:HB	1:A:389:ILE:HG23	1.82	0.60
1:A:60:THR:HG21	1:A:334:LEU:HD23	1.82	0.60
1:A:229:ALA:O	1:A:230:LEU:HB2	2.00	0.60
1:A:99:GLU:O	1:A:361:LEU:HD11	2.02	0.59
1:A:270:ARG:O	1:A:274:LEU:HB2	2.02	0.59
1:A:458:ALA:HB3	1:A:475:LEU:HD23	1.84	0.59
1:A:59:PRO:HD3	1:A:134:ARG:HH11	1.65	0.59
1:A:151:PRO:O	1:A:154:TYR:HB3	2.02	0.59
1:A:85:ALA:CB	1:A:136:VAL:HG13	2.32	0.59
1:A:34:HIS:ND1	1:A:389:ILE:HD11	2.18	0.58
1:A:459:GLU:CG	1:A:475:LEU:HG	2.32	0.58
1:A:473:ALA:CB	1:A:499:LEU:HA	2.33	0.58
1:A:85:ALA:HB3	1:A:136:VAL:HA	1.86	0.58
1:A:162:ARG:NH1	1:A:240:HIS:HB2	2.18	0.58
1:A:291:ARG:HH11	1:A:291:ARG:HG3	1.70	0.57
1:A:551:MET:HE2	1:A:564:ILE:HD11	1.87	0.57
1:A:271:LEU:O	1:A:275:ARG:HB2	2.03	0.57
1:A:521:ASP:HB3	1:A:524:LYS:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:TYR:CD1	1:A:475:LEU:N	2.72	0.57
1:A:281:LEU:HD23	1:A:285:ARG:NH1	2.19	0.57
1:A:286:LEU:CD2	1:A:286:LEU:H	2.18	0.57
1:A:92:TYR:HB3	1:A:96:TYR:CD1	2.40	0.57
1:A:226:GLU:H	1:A:226:GLU:CD	2.07	0.56
1:A:153:GLU:OE2	1:A:252:ARG:NE	2.39	0.56
1:A:281:LEU:HG	1:A:285:ARG:HB3	1.86	0.56
1:A:101:TYR:O	1:A:103:PRO:HD3	2.06	0.56
1:A:59:PRO:HG3	1:A:330:PRO:HG2	1.87	0.56
1:A:218:ASP:HA	1:A:226:GLU:HA	1.88	0.55
1:A:304:SER:OG	1:A:305:GLY:N	2.30	0.55
1:A:192:PHE:O	1:A:202:PHE:HA	2.06	0.55
1:A:60:THR:CG2	1:A:334:LEU:HB3	2.32	0.55
1:A:12:GLU:O	1:A:14:GLN:HG2	2.07	0.54
1:A:207:ASP:O	1:A:209:HIS:N	2.40	0.54
1:A:267:LEU:O	1:A:267:LEU:HG	2.06	0.54
1:A:89:PHE:CD1	1:A:325:LEU:HD22	2.43	0.54
1:A:368:LEU:N	1:A:368:LEU:HD23	2.23	0.54
1:A:551:MET:CE	1:A:564:ILE:HD11	2.37	0.54
1:A:55:GLN:NE2	3:A:780:HOH:O	2.40	0.54
1:A:570:ARG:O	1:A:574:GLN:HG3	2.08	0.54
1:A:152:GLU:O	1:A:156:GLU:HB2	2.08	0.53
1:A:34:HIS:HA	1:A:389:ILE:HD12	1.90	0.53
1:A:174:ARG:HA	1:A:177:VAL:HG23	1.90	0.53
1:A:122:LEU:HA	1:A:125:SER:OG	2.07	0.53
1:A:227:VAL:HG11	1:A:237:GLU:HG3	1.90	0.53
1:A:521:ASP:HB3	1:A:524:LYS:CG	2.39	0.53
1:A:271:LEU:HD13	1:A:283:ALA:HB3	1.91	0.52
1:A:50:SER:O	1:A:53:ILE:HB	2.09	0.52
1:A:19:GLN:HG2	1:A:23:LYS:HE3	1.91	0.52
1:A:363:ASP:HA	3:A:754:HOH:O	2.08	0.52
1:A:60:THR:HB	1:A:334:LEU:O	2.10	0.52
1:A:381:GLU:O	1:A:384:GLN:HG3	2.10	0.52
1:A:92:TYR:HB3	1:A:96:TYR:CE1	2.45	0.52
1:A:358:LYS:O	1:A:362:VAL:HG23	2.10	0.51
1:A:170:ASN:HA	1:A:173:LEU:HB3	1.91	0.51
1:A:474:TYR:HD1	1:A:475:LEU:H	1.58	0.51
1:A:149:GLY:HA3	1:A:248:HIS:O	2.11	0.51
1:A:531:GLU:HG2	1:A:532:ARG:N	2.26	0.50
1:A:266:GLU:OE2	1:A:368:LEU:HD12	2.11	0.50
1:A:50:SER:HB3	1:A:81:PHE:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:HE	1:A:282:GLU:CG	2.24	0.50
1:A:150:SER:OG	1:A:151:PRO:HD2	2.11	0.50
1:A:220:ILE:O	1:A:221:GLU:C	2.50	0.49
1:A:143:SER:HA	1:A:146:TYR:HD1	1.78	0.49
1:A:580:LYS:HG2	1:A:581:HIS:CE1	2.48	0.49
1:A:459:GLU:OE1	1:A:475:LEU:HD11	2.12	0.49
1:A:101:TYR:CE2	1:A:364:HIS:ND1	2.75	0.49
1:A:270:ARG:HD3	1:A:270:ARG:O	2.12	0.49
1:A:37:LEU:HD22	1:A:49:ILE:HD11	1.95	0.49
1:A:116:ASN:O	1:A:118:GLU:N	2.46	0.48
1:A:85:ALA:HB3	1:A:135:ASP:O	2.13	0.48
1:A:281:LEU:HB3	1:A:284:GLN:O	2.12	0.48
1:A:128:SER:HB3	1:A:244:PHE:CD1	2.49	0.48
1:A:275:ARG:HE	1:A:282:GLU:HG3	1.78	0.48
1:A:475:LEU:HD13	1:A:475:LEU:C	2.34	0.48
1:A:48:THR:O	1:A:52:VAL:HG23	2.14	0.48
1:A:578:ASN:HA	1:A:583:ILE:CD1	2.40	0.48
1:A:101:TYR:CD1	1:A:108:TYR:HA	2.47	0.48
1:A:263:ILE:HG21	1:A:294:LEU:HD21	1.95	0.48
1:A:14:GLN:H	1:A:17:GLN:NE2	2.04	0.47
1:A:452:THR:HG21	1:A:457:MET:HG3	1.96	0.47
1:A:281:LEU:HG	1:A:285:ARG:CB	2.44	0.47
1:A:473:ALA:CB	1:A:499:LEU:HG	2.44	0.47
1:A:152:GLU:H	1:A:152:GLU:CD	2.17	0.47
1:A:271:LEU:HD13	1:A:283:ALA:CB	2.45	0.47
1:A:368:LEU:HD23	1:A:368:LEU:H	1.79	0.47
1:A:281:LEU:O	1:A:284:GLN:HG2	2.14	0.47
1:A:543:ARG:HB2	3:A:714:HOH:O	2.15	0.47
1:A:254:GLU:OE2	1:A:257:ARG:NH1	2.46	0.47
1:A:20:ALA:HA	1:A:408:VAL:CG1	2.45	0.47
1:A:268:GLU:O	1:A:271:LEU:N	2.37	0.46
1:A:14:GLN:N	1:A:17:GLN:HE21	2.06	0.46
1:A:333:PHE:H	1:A:333:PHE:HD2	1.61	0.46
1:A:453:LEU:HD12	1:A:524:LYS:HB2	1.98	0.46
1:A:96:TYR:HB3	1:A:112:ASP:O	2.15	0.46
1:A:245:PRO:O	1:A:247:SER:N	2.49	0.46
1:A:459:GLU:N	1:A:475:LEU:HD23	2.31	0.45
1:A:7:LEU:HD21	1:A:47:PHE:CE1	2.52	0.45
1:A:101:TYR:CD2	1:A:364:HIS:ND1	2.81	0.45
1:A:245:PRO:HB3	1:A:250:VAL:HG21	1.97	0.45
1:A:375:ARG:HB2	1:A:376:PRO:CD	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLU:O	1:A:121:LYS:HB3	2.16	0.45
1:A:108:TYR:HD1	1:A:366:PHE:CE2	2.34	0.45
1:A:13:PRO:HA	1:A:17:GLN:HE21	1.81	0.45
1:A:48:THR:HG21	1:A:410:GLN:NE2	2.32	0.45
1:A:101:TYR:OH	1:A:106:ASP:HA	2.17	0.45
1:A:291:ARG:O	1:A:295:GLU:HG3	2.17	0.45
1:A:19:GLN:O	1:A:23:LYS:HB2	2.18	0.44
1:A:196:GLY:O	1:A:197:ASP:CB	2.65	0.44
1:A:492:ARG:HH22	1:A:590:LYS:HB3	1.81	0.44
1:A:17:GLN:N	1:A:18:PRO:HD2	2.33	0.44
1:A:306:ILE:HD11	1:A:313:LEU:HD11	1.98	0.44
1:A:155:ARG:O	1:A:155:ARG:HD3	2.17	0.44
1:A:271:LEU:HA	1:A:271:LEU:HD22	1.79	0.44
1:A:455:LYS:O	1:A:455:LYS:HG2	2.18	0.44
1:A:524:LYS:HD3	1:A:524:LYS:HA	1.73	0.44
1:A:105:THR:O	1:A:106:ASP:C	2.56	0.44
1:A:327:ASP:OD2	1:A:385:LYS:HE3	2.18	0.44
1:A:459:GLU:CB	1:A:475:LEU:HG	2.48	0.44
1:A:150:SER:OG	1:A:152:GLU:OE1	2.36	0.43
1:A:205:SER:O	1:A:207:ASP:N	2.51	0.43
1:A:448:THR:HB	1:A:498:VAL:HG22	2.00	0.43
1:A:578:ASN:OD1	1:A:583:ILE:HB	2.18	0.43
1:A:342:VAL:O	1:A:345:PRO:HD2	2.18	0.43
1:A:447:ARG:O	1:A:514:VAL:HA	2.18	0.43
1:A:52:VAL:O	1:A:56:VAL:HG22	2.18	0.43
1:A:205:SER:HA	1:A:215:PHE:HA	1.99	0.43
1:A:362:VAL:HG12	1:A:362:VAL:O	2.19	0.43
1:A:133:ARG:HH11	1:A:133:ARG:HB3	1.83	0.43
1:A:205:SER:O	1:A:207:ASP:OD1	2.37	0.43
1:A:38:LEU:HD21	1:A:570:ARG:NH2	2.34	0.43
1:A:476:HIS:O	1:A:479:ILE:HG13	2.19	0.43
1:A:108:TYR:HE2	1:A:110:GLU:CG	2.31	0.43
1:A:383:GLU:HA	1:A:386:ILE:HD12	2.00	0.43
1:A:483:GLU:O	1:A:487:ILE:HG13	2.18	0.43
1:A:88:TYR:HB3	1:A:122:LEU:HD13	2.00	0.43
1:A:85:ALA:HB2	1:A:133:ARG:NE	2.34	0.43
1:A:395:THR:HB	1:A:532:ARG:HG2	2.00	0.43
1:A:493:LEU:HG	1:A:592:ILE:HG21	2.00	0.43
1:A:43:THR:HG21	1:A:410:GLN:O	2.19	0.43
1:A:7:LEU:HD12	1:A:80:PHE:HB3	2.01	0.42
1:A:118:GLU:HB3	3:A:762:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LYS:HA	1:A:502:ILE:HD11	2.01	0.42
1:A:306:ILE:O	1:A:307:GLU:C	2.57	0.42
1:A:498:VAL:HG12	1:A:499:LEU:N	2.34	0.42
1:A:87:GLU:HB2	1:A:138:ILE:HG12	2.00	0.42
1:A:124:HIS:O	1:A:128:SER:OG	2.32	0.42
1:A:395:THR:N	1:A:396:PRO:HD3	2.35	0.41
1:A:13:PRO:HA	1:A:17:GLN:NE2	2.35	0.41
1:A:271:LEU:O	1:A:275:ARG:N	2.52	0.41
1:A:522:ALA:HB3	1:A:553:ALA:HB2	2.01	0.41
1:A:17:GLN:N	1:A:18:PRO:CD	2.84	0.41
1:A:492:ARG:HE	1:A:492:ARG:HB2	1.68	0.41
1:A:333:PHE:CD2	1:A:333:PHE:N	2.88	0.41
1:A:434:LEU:HG	1:A:438:ILE:HD12	2.03	0.41
1:A:450:VAL:HG11	1:A:461:LEU:HD21	2.03	0.41
1:A:92:TYR:OH	1:A:119:ILE:HB	2.20	0.41
1:A:286:LEU:HD23	1:A:287:GLU:OE2	2.21	0.41
1:A:61:LEU:HB2	1:A:329:PHE:CZ	2.55	0.41
1:A:364:HIS:O	1:A:366:PHE:N	2.53	0.41
1:A:486:GLU:O	1:A:490:ASP:OD1	2.38	0.41
1:A:98:PRO:O	1:A:99:GLU:C	2.59	0.41
1:A:289:ARG:NH2	1:A:366:PHE:O	2.54	0.41
1:A:281:LEU:HB2	1:A:285:ARG:NH1	2.36	0.40
1:A:288:GLN:O	1:A:292:TYR:HB2	2.21	0.40
1:A:34:HIS:CG	1:A:389:ILE:HD11	2.56	0.40
1:A:70:ALA:O	1:A:139:VAL:HG11	2.21	0.40
1:A:493:LEU:CG	1:A:592:ILE:HD13	2.33	0.40
1:A:593:ARG:HG2	1:A:593:ARG:H	1.73	0.40
1:A:491:LEU:HD12	1:A:496:TYR:O	2.21	0.40
1:A:528:LEU:HD23	1:A:528:LEU:HA	1.89	0.40
1:A:360:VAL:O	1:A:363:ASP:HB2	2.21	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	
1	A	584/658 (89%)	475 (81%)	69 (12%)	40 (7%)	1	1

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	GLU
1	A	117	ASP
1	A	181	TYR
1	A	199	VAL
1	A	208	GLU
1	A	210	CYS
1	A	213	VAL
1	A	215	PHE
1	A	220	ILE
1	A	277	GLN
1	A	282	GLU
1	A	304	SER
1	A	365	GLY
1	A	95	TYR
1	A	168	GLU
1	A	197	ASP
1	A	206	ARG
1	A	209	HIS
1	A	230	LEU
1	A	236	GLY
1	A	283	ALA
1	A	285	ARG
1	A	96	TYR
1	A	189	ARG
1	A	194	VAL
1	A	195	ARG
1	A	203	PRO
1	A	205	SER
1	A	246	ALA
1	A	475	LEU
1	A	103	PRO
1	A	235	LEU
1	A	284	GLN
1	A	151	PRO
1	A	191	THR

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Mol	Chain	Res	Type
1	A	211	ILE
1	A	21	ILE
1	A	202	PHE
1	A	179	ILE
1	A	479	ILE

### 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	482/569 (85%)	394 (82%)	88 (18%)	<b>2</b> <b>3</b>

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	14	GLN
1	A	17	GLN
1	A	19	GLN
1	A	38	LEU
1	A	50	SER
1	A	55	GLN
1	A	56	VAL
1	A	58	LYS
1	A	68	THR
1	A	91	SER
1	A	96	TYR
1	A	104	GLN
1	A	105	THR
1	A	107	THR
1	A	114	LYS
1	A	117	ASP
1	A	122	LEU
1	A	128	SER
1	A	133	ARG
1	A	134	ARG

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Mol	Chain	Res	Type
1	A	136	VAL
1	A	155	ARG
1	A	156	GLU
1	A	162	ARG
1	A	166	GLU
1	A	167	ILE
1	A	169	ARG
1	A	173	LEU
1	A	176	LEU
1	A	177	VAL
1	A	206	ARG
1	A	208	GLU
1	A	226	GLU
1	A	228	ASP
1	A	230	LEU
1	A	231	THR
1	A	235	LEU
1	A	237	GLU
1	A	239	GLU
1	A	250	VAL
1	A	270	ARG
1	A	271	LEU
1	A	274	LEU
1	A	275	ARG
1	A	281	LEU
1	A	285	ARG
1	A	286	LEU
1	A	296	MET
1	A	300	MET
1	A	302	PHE
1	A	303	CYS
1	A	315	LEU
1	A	316	ARG
1	A	333	PHE
1	A	346	GLN
1	A	347	LEU
1	A	348	ARG
1	A	368	LEU
1	A	389	ILE
1	A	404	SER
1	A	410	GLN
1	A	441	ARG

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Mol	Chain	Res	Type
1	A	442	VAL
1	A	444	ARG
1	A	453	LEU
1	A	460	ASP
1	A	464	TYR
1	A	466	LYS
1	A	467	GLU
1	A	475	LEU
1	A	479	ILE
1	A	482	LEU
1	A	484	ARG
1	A	485	ILE
1	A	486	GLU
1	A	488	ILE
1	A	493	LEU
1	A	507	GLU
1	A	520	LEU
1	A	525	GLU
1	A	540	ARG
1	A	576	GLU
1	A	588	VAL
1	A	589	LYS
1	A	593	ARG
1	A	594	ASP
1	A	595	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	14	GLN
1	A	17	GLN
1	A	19	GLN
1	A	240	HIS
1	A	374	ASN
1	A	384	GLN
1	A	410	GLN

### 5.3.3 RNA ⓘ

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	590/658 (89%)	0.26	46 (7%) 16 11	29, 67, 101, 101	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	TYR	7.3
1	A	93	TYR	7.0
1	A	235	LEU	4.3
1	A	2	GLU	4.2
1	A	195	ARG	4.1
1	A	186	ILE	4.0
1	A	94	ASP	3.9
1	A	165	MET	3.8
1	A	197	ASP	3.7
1	A	237	GLU	3.7
1	A	199	VAL	3.6
1	A	236	GLY	3.6
1	A	108	TYR	3.4
1	A	164	GLY	3.3
1	A	475	LEU	3.2
1	A	473	ALA	3.2
1	A	163	VAL	3.1
1	A	479	ILE	3.0
1	A	114	LYS	2.9
1	A	482	LEU	2.9
1	A	499	LEU	2.8
1	A	593	ARG	2.8
1	A	591	GLU	2.7
1	A	500	VAL	2.6
1	A	169	ARG	2.6
1	A	185	ASP	2.6
1	A	594	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	501	GLY	2.5
1	A	196	GLY	2.5
1	A	118	GLU	2.5
1	A	97	GLN	2.4
1	A	113	ALA	2.3
1	A	189	ARG	2.3
1	A	498	VAL	2.2
1	A	243	ILE	2.2
1	A	478	GLU	2.2
1	A	233	LYS	2.2
1	A	200	GLU	2.2
1	A	225	ALA	2.1
1	A	112	ASP	2.1
1	A	278	GLY	2.1
1	A	174	ARG	2.1
1	A	115	ILE	2.1
1	A	190	GLY	2.1
1	A	191	THR	2.0
1	A	61	LEU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	A	702	1/1	0.80	0.21	-	65,65,65,65	1
2	ZN	A	701	1/1	0.99	0.09	-	76,76,76,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.