



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:18 PM UTC

PDB ID : 1D9X / pdb_00001d9x
Title : CRYSTAL STRUCTURE OF THE DNA REPAIR PROTEIN UVRB
Authors : Theis, K.; Chen, P.J.; Skovvaga, 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

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

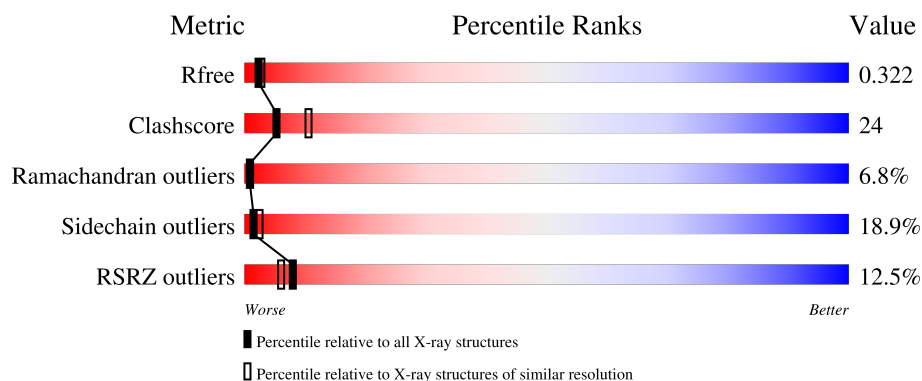
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	658	

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 (CCD ID: ZN) (formula: Zn).

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

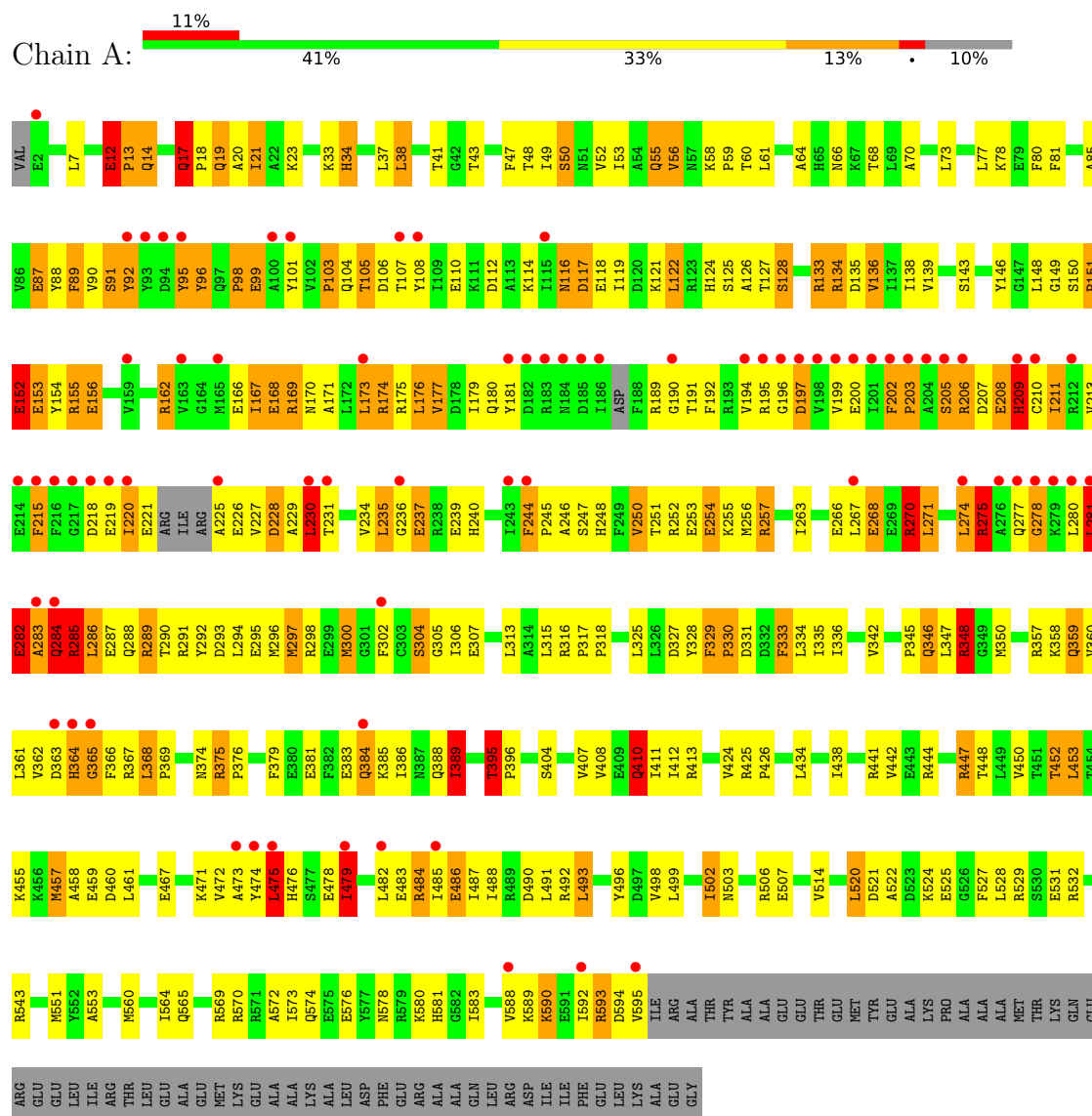
- Molecule 3 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: EXCINUCLEASE UVRABC COMPONENT UVRB



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.21 Å 150.21 Å 79.52 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.60) 99.7 (20.00-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.59 Å)	Xtriage
Refinement program	REFMAC, X-PLOR	Depositor
R, R_{free}	0.256 , 0.324 0.254 , 0.322	Depositor DCC
R_{free} test set	1632 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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

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	1.02	1/4705 (0.0%)	1.83	100/6365 (1.6%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	GLU	N-CA	-5.42	1.39	1.46

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	ARG	CD-NE-CZ	12.15	141.41	124.40
1	A	413	ARG	CD-NE-CZ	10.03	138.44	124.40
1	A	520	LEU	N-CA-C	9.61	124.80	112.89
1	A	502	ILE	N-CA-C	-8.46	103.64	111.67
1	A	203	PRO	N-CA-CB	7.86	111.50	103.25
1	A	281	LEU	N-CA-C	-7.85	102.65	113.56
1	A	379	PHE	CA-CB-CG	-7.69	106.11	113.80
1	A	441	ARG	NE-CZ-NH2	-7.65	112.31	119.20
1	A	441	ARG	NH1-CZ-NH2	7.55	129.11	119.30
1	A	348	ARG	CD-NE-CZ	7.48	134.87	124.40
1	A	116	ASN	CA-C-N	7.47	135.81	121.54
1	A	116	ASN	C-N-CA	7.47	135.81	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	LEU	CA-C-N	7.21	135.30	121.54
1	A	281	LEU	C-N-CA	7.21	135.30	121.54
1	A	17	GLN	CB-CG-CD	6.93	124.38	112.60
1	A	66	ASN	CA-CB-CG	6.90	119.50	112.60
1	A	98	PRO	N-CA-CB	6.75	107.25	102.79
1	A	289	ARG	CD-NE-CZ	6.74	133.84	124.40
1	A	209	HIS	CA-C-N	6.72	134.37	121.54
1	A	209	HIS	C-N-CA	6.72	134.37	121.54
1	A	127	THR	CA-CB-OG1	6.70	119.64	109.60
1	A	175	ARG	CA-C-N	6.65	131.95	120.58
1	A	175	ARG	C-N-CA	6.65	131.95	120.58
1	A	280	LEU	CA-C-O	6.52	130.30	122.41
1	A	190	GLY	CA-C-N	6.50	133.96	121.54
1	A	190	GLY	C-N-CA	6.50	133.96	121.54
1	A	329	PHE	CA-C-N	6.50	126.88	119.92
1	A	329	PHE	C-N-CA	6.50	126.88	119.92
1	A	180	GLN	CA-C-N	6.50	133.95	121.54
1	A	180	GLN	C-N-CA	6.50	133.95	121.54
1	A	278	GLY	N-CA-C	6.46	122.51	111.98
1	A	410	GLN	CB-CG-CD	6.44	123.55	112.60
1	A	293	ASP	CA-CB-CG	6.42	119.03	112.60
1	A	298	ARG	NE-CZ-NH2	-6.29	113.54	119.20
1	A	234	VAL	O-C-N	-6.25	117.15	122.65
1	A	64	ALA	CA-C-O	-6.25	114.34	121.72
1	A	95	TYR	CA-C-N	6.24	133.46	121.54
1	A	95	TYR	C-N-CA	6.24	133.46	121.54
1	A	441	ARG	CA-C-N	6.22	128.40	120.56
1	A	441	ARG	C-N-CA	6.22	128.40	120.56
1	A	395	THR	CA-C-N	6.13	126.16	119.90
1	A	395	THR	C-N-CA	6.13	126.16	119.90
1	A	330	PRO	N-CA-CB	6.09	109.12	103.39
1	A	529	ARG	CD-NE-CZ	-6.07	115.91	124.40
1	A	257	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	A	284	GLN	OE1-CD-NE2	5.99	128.59	122.60
1	A	89	PHE	CA-CB-CG	5.94	119.74	113.80
1	A	331	ASP	N-CA-C	5.94	118.54	111.71
1	A	12	GLU	N-CA-C	5.86	115.05	108.25
1	A	346	GLN	CA-C-N	5.86	129.61	120.82
1	A	346	GLN	C-N-CA	5.86	129.61	120.82
1	A	300	MET	CA-CB-CG	5.86	125.81	114.10
1	A	34	HIS	CA-CB-CG	5.78	119.58	113.80
1	A	367	ARG	CA-C-O	-5.76	115.07	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ILE	CB-CA-C	-5.73	102.00	110.82
1	A	87	GLU	N-CA-C	5.73	118.40	109.52
1	A	389	ILE	CA-CB-CG2	5.70	120.18	110.50
1	A	298	ARG	CD-NE-CZ	-5.69	116.43	124.40
1	A	457	MET	N-CA-C	-5.57	105.21	112.23
1	A	318	PRO	N-CA-CB	5.56	108.26	103.31
1	A	317	PRO	O-C-N	-5.53	118.55	121.15
1	A	169	ARG	N-CA-C	-5.51	106.32	113.16
1	A	374	ASN	OD1-CG-ND2	5.51	128.11	122.60
1	A	412	ILE	N-CA-C	5.50	116.30	107.73
1	A	92	TYR	CA-C-N	5.48	128.64	120.31
1	A	92	TYR	C-N-CA	5.48	128.64	120.31
1	A	275	ARG	CD-NE-CZ	5.46	132.04	124.40
1	A	346	GLN	O-C-N	-5.46	116.45	122.07
1	A	357	ARG	CA-C-N	5.45	131.73	122.36
1	A	357	ARG	C-N-CA	5.45	131.73	122.36
1	A	41	THR	N-CA-C	-5.44	103.35	110.53
1	A	425	ARG	CA-C-N	5.42	125.40	120.03
1	A	425	ARG	C-N-CA	5.42	125.40	120.03
1	A	174	ARG	CA-C-N	5.39	128.05	120.28
1	A	174	ARG	C-N-CA	5.39	128.05	120.28
1	A	13	PRO	N-CA-CB	5.39	108.91	103.25
1	A	384	GLN	CB-CG-CD	5.37	121.72	112.60
1	A	426	PRO	N-CA-CB	5.33	108.97	103.38
1	A	375	ARG	N-CA-CB	-5.32	104.59	111.35
1	A	228	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	254	GLU	CA-C-O	-5.31	114.92	120.55
1	A	369	PRO	CA-C-N	5.30	128.12	120.38
1	A	369	PRO	C-N-CA	5.30	128.12	120.38
1	A	388	GLN	OE1-CD-NE2	5.29	127.89	122.60
1	A	447	ARG	NE-CZ-NH1	5.26	126.77	121.50
1	A	211	ILE	CA-C-N	5.24	129.34	122.06
1	A	211	ILE	C-N-CA	5.24	129.34	122.06
1	A	270	ARG	NE-CZ-NH2	-5.24	114.49	119.20
1	A	357	ARG	CB-CG-CD	5.24	123.34	111.30
1	A	244	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	364	HIS	CA-C-N	5.17	131.54	121.41
1	A	364	HIS	C-N-CA	5.17	131.54	121.41
1	A	527	PHE	N-CA-C	-5.14	105.59	111.14
1	A	369	PRO	N-CA-CB	5.13	108.74	103.15
1	A	176	LEU	N-CA-C	5.10	117.96	111.69
1	A	572	ALA	O-C-N	5.09	127.32	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	GLN	N-CA-C	-5.06	105.76	111.28
1	A	569	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	A	413	ARG	CA-C-N	5.02	124.81	119.28
1	A	413	ARG	C-N-CA	5.02	124.81	119.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	GLU	Mainchain
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	224	0
2	A	2	0	0	0	0
3	A	83	0	0	6	0
All	All	4717	0	4577	224	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 24.

All (224) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:551:MET:HE1	1:A:564:ILE:HD11	1.74	0.70
1:A:274:LEU:HD22	1:A:283:ALA:HA	1.73	0.70
1:A:267:LEU:HD13	1:A:290:THR:HG21	1.75	0.69
1:A:239:GLU:CD	1:A:239:GLU:H	2.01	0.69
1:A:455:LYS:O	1:A:475:LEU:HD21	1.93	0.68
1:A:479:ILE:HD12	1:A:479:ILE:H	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:90:VAL:HG22	1:A:91:SER:H	1.60	0.65
1:A:503:ASN:O	1:A:506:ARG:HG3	1.96	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:73:LEU:O	1:A:77:LEU:HB2	1.97	0.64
1:A:284:GLN:O	1:A:285:ARG:CB	2.45	0.64
1:A:475:LEU:O	1:A:475:LEU:HD22	1.98	0.63
1:A:87:GLU:HG3	1:A:126:ALA:HA	1.80	0.62
1:A:286:LEU:H	1:A:286:LEU:HD23	1.63	0.62
1:A:226:GLU:CD	1:A:226:GLU:H	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PRO:HD3	1:A:134:ARG:HH11	1.65	0.59
1:A:458:ALA:HB3	1:A:475:LEU:HD23	1.84	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: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
1:A:474:TYR:CD1	1:A:475:LEU:N	2.72	0.57
1:A:92:TYR:HB3	1:A:96:TYR:CD1	2.40	0.57
1:A:281:LEU:HD23	1:A:285:ARG:NH1	2.19	0.57
1:A:286:LEU:H	1:A:286:LEU:CD2	2.18	0.57
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:59:PRO:HG3	1:A:330:PRO:HG2	1.87	0.56
1:A:101:TYR:O	1:A:103:PRO:HD3	2.06	0.56
1:A:551:MET:HE3	1:A:560:MET:HE3	1.88	0.55
1:A:218:ASP:HA	1:A:226:GLU:HA	1.88	0.55
1:A:424:VAL:HG22	1:A:551:MET:HE2	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:89:PHE:CD1	1:A:325:LEU:HD22	2.43	0.54
1:A:220:ILE:O	1:A:221:GLU:C	2.50	0.54
1:A:267:LEU:HG	1:A:267:LEU:O	2.06	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:34:HIS:HA	1:A:389:ILE:HD12	1.90	0.53
1:A:152:GLU:O	1:A:156:GLU:HB2	2.08	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:475:LEU:C	1:A:475:LEU:HD13	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:152:GLU:CD	1:A:152:GLU:H	2.17	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
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:263:ILE:HD12	1:A:297:MET:HE1	1.94	0.50
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:37:LEU:HD22	1:A:49:ILE:HD11	1.95	0.49
1:A:101:TYR:CE2	1:A:364:HIS:ND1	2.75	0.49
1:A:270:ARG:O	1:A:270:ARG:HD3	2.12	0.49
1:A:85:ALA:HB3	1:A:135:ASP:O	2.13	0.48
1:A:116:ASN:O	1:A:118:GLU:N	2.46	0.48
1:A:281:LEU:HB3	1:A:284:GLN:O	2.12	0.48
1:A:48:THR:O	1:A:52:VAL:HG23	2.14	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:578:ASN:HA	1:A:583:ILE:CD1	2.40	0.48
1:A:263:ILE:CD1	1:A:297:MET:HE1	2.43	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:105:THR:O	1:A:106:ASP:C	2.56	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:271:LEU:HD13	1:A:283:ALA:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ILE:O	1:A:307:GLU:C	2.57	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:20:ALA:HA	1:A:408:VAL:CG1	2.45	0.47
1:A:254:GLU:OE2	1:A:257:ARG:NH1	2.46	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:98:PRO:O	1:A:99:GLU:C	2.59	0.46
1:A:245:PRO:O	1:A:247:SER:N	2.49	0.46
1:A:251:THR:HB	1:A:256:MET:HE2	1.97	0.46
1:A:7:LEU:HD21	1:A:47:PHE:CE1	2.52	0.45
1:A:459:GLU:N	1:A:475:LEU:HD23	2.31	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
1:A:108:TYR:HD1	1:A:366:PHE:CE2	2.34	0.45
1:A:118:GLU:O	1:A:121:LYS:HB3	2.16	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:167:ILE:O	1:A:168:GLU:C	2.60	0.44
1:A:196:GLY:O	1:A:197:ASP:CB	2.65	0.44
1:A:350:MET:HE2	1:A:350:MET:HA	1.99	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:HD22	1:A:271:LEU:HA	1.79	0.44
1:A:455:LYS:O	1:A:455:LYS:HG2	2.18	0.44
1:A:524:LYS:HA	1:A:524:LYS:HD3	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:ASN:OD1	1:A:583:ILE:HB	2.18	0.43
1:A:52:VAL:O	1:A:56:VAL:HG22	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:205:SER:HA	1:A:215:PHE:HA	1.99	0.43
1:A:362:VAL:O	1:A:362:VAL:HG12	2.19	0.43
1:A:38:LEU:HD21	1:A:570:ARG:NH2	2.34	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: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:88:TYR:HB3	1:A:122:LEU:HD13	2.00	0.43
1:A:483:GLU:O	1:A:487:ILE:HG13	2.18	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
1:A:455:LYS:HA	1:A:502:ILE:HD11	2.01	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:252:ARG:O	1:A:253:GLU:C	2.62	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:342:VAL:C	1:A:345:PRO:HD2	2.45	0.41
1:A:492:ARG:HE	1:A:492:ARG:HB2	1.68	0.41
1:A:92:TYR:OH	1:A:119:ILE:HB	2.20	0.41
1:A:333:PHE:N	1:A:333:PHE:CD2	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:61:LEU:HB2	1:A:329:PHE:CZ	2.55	0.41
1:A:286:LEU:HD23	1:A:287:GLU:OE2	2.21	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:289:ARG:NH2	1:A:366:PHE:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:MET:HE3	1:A:560:MET:HG2	2.02	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:H	1:A:593:ARG:HG2	1.73	0.40
1:A:20:ALA:O	1:A:21:ILE:C	2.65	0.40
1:A:103:PRO:O	1:A:104:GLN:C	2.64	0.40
1:A:491:LEU:HD12	1:A:496:TYR:O	2.21	0.40
1:A:528:LEU:HA	1:A:528:LEU:HD23	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%)	 

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

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Mol	Chain	Res	Type
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
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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	482/569 (85%)	391 (81%)	91 (19%)	1 2

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLU
1	A	14	GLN
1	A	17	GLN
1	A	19	GLN
1	A	33	LYS
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	78	LYS
1	A	91	SER
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
1	A	136	VAL
1	A	152	GLU
1	A	153	GLU
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

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Mol	Chain	Res	Type
1	A	228	ASP
1	A	230	LEU
1	A	231	THR
1	A	235	LEU
1	A	237	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	297	MET
1	A	300	MET
1	A	302	PHE
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	359	GLN
1	A	368	LEU
1	A	389	ILE
1	A	395	THR
1	A	404	SER
1	A	407	VAL
1	A	410	GLN
1	A	442	VAL
1	A	444	ARG
1	A	452	THR
1	A	453	LEU
1	A	460	ASP
1	A	467	GLU
1	A	472	VAL
1	A	475	LEU
1	A	479	ILE
1	A	482	LEU
1	A	484	ARG
1	A	485	ILE

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Mol	Chain	Res	Type
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	565	GLN
1	A	576	GLU
1	A	588	VAL
1	A	589	LYS
1	A	590	LYS
1	A	593	ARG
1	A	594	ASP
1	A	595	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	17	GLN
1	A	19	GLN
1	A	57	ASN
1	A	124	HIS
1	A	240	HIS
1	A	261	GLN
1	A	312	HIS
1	A	374	ASN
1	A	384	GLN
1	A	410	GLN
1	A	445	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 oligosaccharides 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, 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	590/658 (89%)	0.58	74 (12%) 8 6	29, 67, 101, 101	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	93	TYR	8.2
1	A	95	TYR	5.1
1	A	278	GLY	4.4
1	A	183	ARG	4.2
1	A	280	LEU	3.8
1	A	210	CYS	3.8
1	A	220	ILE	3.8
1	A	203	PRO	3.8
1	A	216	PHE	3.7
1	A	94	ASP	3.7
1	A	182	ASP	3.7
1	A	473	ALA	3.7
1	A	595	VAL	3.7
1	A	108	TYR	3.6
1	A	281	LEU	3.6
1	A	195	ARG	3.5
1	A	185	ASP	3.5
1	A	190	GLY	3.5
1	A	186	ILE	3.5
1	A	205	SER	3.4
1	A	365	GLY	3.3
1	A	199	VAL	3.3
1	A	204	ALA	3.3
1	A	212	ARG	3.3
1	A	92	TYR	3.2
1	A	197	ASP	3.2
1	A	217	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	225	ALA	3.1
1	A	194	VAL	3.1
1	A	276	ALA	3.0
1	A	284	GLN	3.0
1	A	236	GLY	3.0
1	A	475	LEU	2.9
1	A	198	VAL	2.9
1	A	2	GLU	2.8
1	A	479	ILE	2.8
1	A	202	PHE	2.7
1	A	159	VAL	2.7
1	A	218	ASP	2.7
1	A	279	LYS	2.6
1	A	173	LEU	2.6
1	A	101	TYR	2.6
1	A	215	PHE	2.6
1	A	277	GLN	2.6
1	A	165	MET	2.5
1	A	196	GLY	2.5
1	A	302	PHE	2.5
1	A	364	HIS	2.5
1	A	219	GLU	2.5
1	A	283	ALA	2.5
1	A	230	LEU	2.4
1	A	482	LEU	2.4
1	A	267	LEU	2.4
1	A	214	GLU	2.4
1	A	181	TYR	2.3
1	A	474	TYR	2.3
1	A	592	ILE	2.3
1	A	231	THR	2.3
1	A	206	ARG	2.3
1	A	274	LEU	2.2
1	A	201	ILE	2.2
1	A	363	ASP	2.2
1	A	588	VAL	2.2
1	A	200	GLU	2.2
1	A	184	ASN	2.2
1	A	209	HIS	2.2
1	A	115	ILE	2.1
1	A	163	VAL	2.1
1	A	100	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	244	PHE	2.1
1	A	485	ILE	2.1
1	A	107	THR	2.0
1	A	384	GLN	2.0
1	A	243	ILE	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](#)

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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å ²)	Q<0.9
2	ZN	A	702	1/1	0.77	0.23	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.