



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:05 AM UTC

PDB ID : 4NZV / pdb_00004nzh
Title : DNA Double-Strand Break Repair Pathway Choice Is Directed by Distinct MRE11 Nuclease Activities
Authors : Shibata, A.; Moiani, D.; Arvai, A.S.; Perry, J.; Harding, S.M.; Genois, M.; Maity, R.; Rossum-Fikkert, S.; Kertokallio, A.; Romoli, F.; Ismail, A.; Ismalaj, E.; Petricci, E.; Neale, M.J.; Bristow, R.G.; Masson, J.; Wyman, C.; Jeggo, P.A.; Tainer, J.A.
Deposited on : 2013-12-12
Resolution : 1.90 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

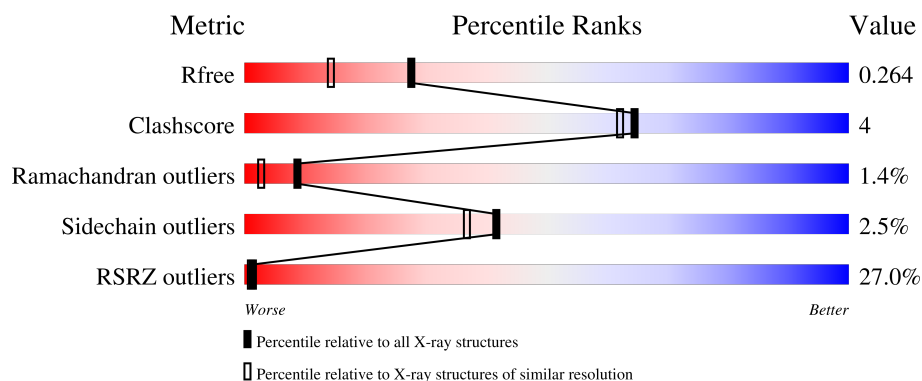
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	336	20% 88% 8% ..
1	B	336	32% 82% 13% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5532 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 Exonuclease, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	1	0
			2639	1695	452	486	6			
1	B	324	Total	C	N	O	S	0	0	0
			2584	1663	439	476	6			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q9X1X0
A	-10	GLY	-	expression tag	UNP Q9X1X0
A	-9	SER	-	expression tag	UNP Q9X1X0
A	-8	ASP	-	expression tag	UNP Q9X1X0
A	-7	LYS	-	expression tag	UNP Q9X1X0
A	-6	ILE	-	expression tag	UNP Q9X1X0
A	-5	HIS	-	expression tag	UNP Q9X1X0
A	-4	HIS	-	expression tag	UNP Q9X1X0
A	-3	HIS	-	expression tag	UNP Q9X1X0
A	-2	HIS	-	expression tag	UNP Q9X1X0
A	-1	HIS	-	expression tag	UNP Q9X1X0
A	0	HIS	-	expression tag	UNP Q9X1X0
A	1	VAL	-	expression tag	UNP Q9X1X0
B	-11	MET	-	initiating methionine	UNP Q9X1X0
B	-10	GLY	-	expression tag	UNP Q9X1X0
B	-9	SER	-	expression tag	UNP Q9X1X0
B	-8	ASP	-	expression tag	UNP Q9X1X0
B	-7	LYS	-	expression tag	UNP Q9X1X0
B	-6	ILE	-	expression tag	UNP Q9X1X0
B	-5	HIS	-	expression tag	UNP Q9X1X0
B	-4	HIS	-	expression tag	UNP Q9X1X0
B	-3	HIS	-	expression tag	UNP Q9X1X0
B	-2	HIS	-	expression tag	UNP Q9X1X0
B	-1	HIS	-	expression tag	UNP Q9X1X0
B	0	HIS	-	expression tag	UNP Q9X1X0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	VAL	-	expression tag	UNP Q9X1X0

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mn 2	0	0
2	B	2	Total 2	Mn 2	0	0

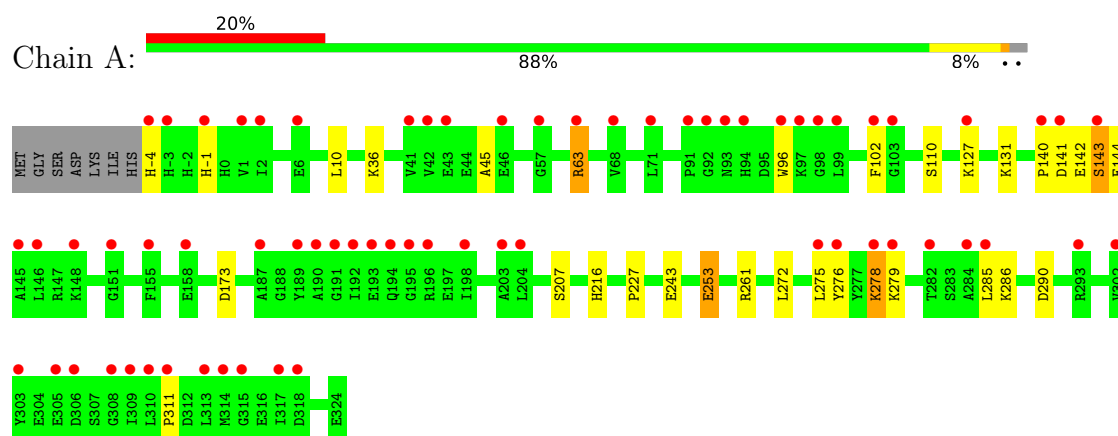
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	154	Total 154	O 154	0	0
3	B	151	Total 151	O 151	0	0

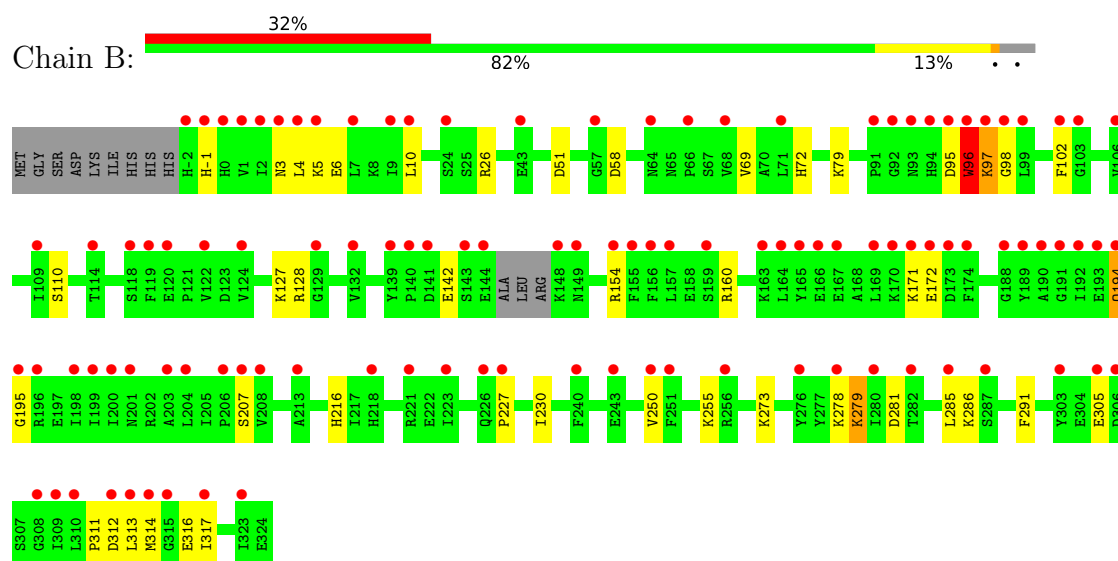
3 Residue-property plots [i](#)

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: Exonuclease, putative



- Molecule 1: Exonuclease, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.12Å 109.95Å 76.92Å 90.00° 100.21° 90.00°	Depositor
Resolution (Å)	44.48 – 1.90 44.48 – 1.90	Depositor EDS
% Data completeness (in resolution range)	89.9 (44.48-1.90) 90.0 (44.48-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.231 , 0.266 0.231 , 0.264	Depositor DCC
R_{free} test set	2000 reflections (3.32%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.58$, $\langle L^2 \rangle = 0.43$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5532	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4210e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.34	0/2704	0.72	1/3660 (0.0%)
1	B	0.35	0/2643	0.73	1/3576 (0.0%)
All	All	0.34	0/5347	0.73	2/7236 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	GLU	N-CA-C	-5.47	105.48	111.82
1	B	194	GLN	N-CA-C	5.45	118.05	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2639	0	2621	15	0
1	B	2584	0	2562	27	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	154	0	0	2	0
3	B	151	0	0	7	0
All	All	5532	0	5183	41	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 4.

All (41) 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:B:95:ASP:O	1:B:97:LYS:N	2.21	0.73
1:B:3:ASN:O	1:B:5:LYS:N	2.20	0.73
1:B:-1:HIS:HB2	1:B:128:ARG:HA	1.76	0.66
1:B:72:HIS:ND1	3:B:572:HOH:O	2.28	0.66
1:B:279:LYS:HB3	1:B:305:GLU:HB2	1.77	0.66
1:B:285:LEU:HD21	1:B:311:PRO:HG3	1.79	0.64
1:B:154:ARG:NH1	3:B:559:HOH:O	2.32	0.63
1:B:160:ARG:NH1	3:B:564:HOH:O	2.30	0.63
1:A:285:LEU:HD21	1:A:311:PRO:HG3	1.83	0.61
1:B:26:ARG:NH2	1:B:314:MET:O	2.35	0.60
1:A:10:LEU:HD22	1:A:45:ALA:HB2	1.84	0.60
1:A:141:ASP:O	1:A:143:SER:N	2.35	0.59
1:B:110:SER:O	3:B:537:HOH:O	2.17	0.59
1:B:6:GLU:HG2	1:B:255:LYS:HG2	1.86	0.58
1:B:194:GLN:N	1:B:195:GLY:HA2	2.19	0.58
1:B:278:LYS:H	1:B:278:LYS:HD3	1.70	0.55
1:A:207:SER:HA	1:A:227:PRO:HD3	1.91	0.53
1:B:316:GLU:HG3	1:B:317:ILE:HG13	1.90	0.53
1:A:110:SER:O	3:A:518:HOH:O	2.19	0.50
1:A:253:GLU:HB3	1:A:261:ARG:HG3	1.94	0.49
1:A:63:ARG:NE	1:A:63:ARG:H	2.11	0.48
1:A:102:PHE:HD2	1:B:102:PHE:HD1	1.62	0.47
1:B:273:LYS:HG2	1:B:291:PHE:CZ	2.50	0.47
1:B:207:SER:HA	1:B:227:PRO:HD3	1.95	0.47
1:A:131:LYS:O	1:A:173:ASP:HB2	2.15	0.47
1:A:278:LYS:HE2	1:A:279:LYS:H	1.80	0.47
1:B:58:ASP:OD2	3:B:507:HOH:O	2.21	0.44
1:B:230:ILE:HG21	1:B:250:VAL:HG21	2.00	0.44
1:A:243:GLU:HG3	1:A:272:LEU:HB2	1.98	0.44
1:A:36:LYS:NZ	3:A:640:HOH:O	2.49	0.43
1:A:96:TRP:CD1	1:A:96:TRP:H	2.36	0.43
1:B:127:LYS:NZ	3:B:615:HOH:O	2.50	0.43
1:A:286:LYS:NZ	1:A:290:ASP:OD2	2.52	0.42
1:B:51:ASP:HA	1:B:127:LYS:HB3	2.02	0.42
1:B:311:PRO:O	1:B:313:LEU:N	2.53	0.42
1:A:-1:HIS:HE1	1:A:127:LYS:HE2	1.85	0.42
1:B:69:VAL:HG23	3:B:613:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ASP:OD2	1:B:281:ASP:N	2.52	0.41
1:B:278:LYS:HG2	1:B:279:LYS:H	1.85	0.41
1:B:96:TRP:C	1:B:98:GLY:H	2.29	0.40
1:B:278:LYS:H	1:B:278:LYS:CD	2.32	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	328/336 (98%)	320 (98%)	5 (2%)	3 (1%)	14	6
1	B	320/336 (95%)	303 (95%)	11 (3%)	6 (2%)	6	1
All	All	648/672 (96%)	623 (96%)	16 (2%)	9 (1%)	9	3

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	LEU
1	B	96	TRP
1	A	142	GLU
1	A	216	HIS
1	B	171	LYS
1	B	216	HIS
1	B	142	GLU
1	B	312	ASP
1	A	140	PRO

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	285/298 (96%)	278 (98%)	7 (2%)	42	37
1	B	277/298 (93%)	270 (98%)	7 (2%)	42	37
All	All	562/596 (94%)	548 (98%)	14 (2%)	42	37

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-4	HIS
1	A	63	ARG
1	A	143	SER
1	A	253	GLU
1	A	275	LEU
1	A	276	TYR
1	A	278	LYS
1	B	10	LEU
1	B	79	LYS
1	B	96	TRP
1	B	97	LYS
1	B	172	GLU
1	B	279	LYS
1	B	286	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	B	64	ASN
1	B	226	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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	329/336 (97%)	1.24	67 (20%) 3 2	26, 42, 102, 142	1 (0%)
1	B	324/336 (96%)	1.73	109 (33%) 1 1	27, 47, 109, 148	0
All	All	653/672 (97%)	1.48	176 (26%) 1 1	26, 44, 108, 148	1 (0%)

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	TYR	11.7
1	B	2	ILE	9.6
1	B	190	ALA	7.6
1	B	1	VAL	7.5
1	B	96	TRP	7.1
1	A	146	LEU	6.8
1	B	192	ILE	6.8
1	B	143	SER	6.6
1	A	-3	HIS	6.4
1	B	98	GLY	6.3
1	B	4	LEU	5.9
1	B	191	GLY	5.8
1	A	191	GLY	5.8
1	B	57	GLY	5.2
1	B	99	LEU	5.1
1	A	98	GLY	5.1
1	A	96	TRP	4.8
1	B	170	LYS	4.7
1	B	189	TYR	4.6
1	A	145	ALA	4.5
1	B	3	ASN	4.4
1	B	93	ASN	4.4
1	B	195	GLY	4.4
1	A	192	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	169	LEU	4.2
1	A	190	ALA	4.2
1	A	141	ASP	4.2
1	B	196	ARG	4.2
1	B	226	GLN	4.2
1	A	99	LEU	4.1
1	B	155	PHE	4.1
1	B	144	GLU	4.1
1	B	97	LYS	4.1
1	A	103	GLY	4.0
1	B	-1	HIS	4.0
1	B	278	LYS	3.9
1	B	-2	HIS	3.8
1	A	189	TYR	3.8
1	A	-4	HIS	3.8
1	B	323	ILE	3.7
1	A	193	GLU	3.7
1	B	167	GLU	3.6
1	B	203	ALA	3.6
1	B	303	TYR	3.6
1	B	309	ILE	3.6
1	B	276	TYR	3.6
1	A	43	GLU	3.6
1	B	139	TYR	3.5
1	A	2	ILE	3.5
1	A	194	GLN	3.5
1	B	122	VAL	3.4
1	B	132	VAL	3.4
1	A	-1	HIS	3.4
1	B	103	GLY	3.4
1	B	154	ARG	3.4
1	B	208	VAL	3.4
1	B	159	SER	3.3
1	B	166	GLU	3.3
1	A	279	LYS	3.3
1	B	102	PHE	3.3
1	A	317	ILE	3.2
1	A	315	GLY	3.2
1	A	148	LYS	3.2
1	B	10	LEU	3.2
1	B	156	PHE	3.2
1	B	317	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	91	PRO	3.2
1	A	313	LEU	3.2
1	B	92	GLY	3.2
1	A	155	PHE	3.1
1	B	64	ASN	3.1
1	B	308	GLY	3.1
1	B	194	GLN	3.1
1	A	92	GLY	3.1
1	A	284	ALA	3.1
1	B	165	TYR	3.0
1	B	91	PRO	3.0
1	B	94	HIS	3.0
1	B	305	GLU	3.0
1	A	140	PRO	3.0
1	B	172	GLU	3.0
1	B	171	LYS	2.9
1	B	285	LEU	2.9
1	B	141	ASP	2.9
1	A	57	GLY	2.9
1	B	120	GLU	2.9
1	B	313	LEU	2.9
1	A	93	ASN	2.8
1	A	94	HIS	2.8
1	B	174	PHE	2.8
1	B	207	SER	2.8
1	B	7	LEU	2.8
1	B	149	ASN	2.8
1	B	280	ILE	2.8
1	B	315	GLY	2.7
1	A	204	LEU	2.7
1	B	227	PRO	2.7
1	B	206	PRO	2.7
1	A	151	GLY	2.7
1	A	195	GLY	2.7
1	A	285	LEU	2.7
1	B	250	VAL	2.7
1	A	305	GLU	2.6
1	A	278	LYS	2.6
1	B	9	ILE	2.6
1	B	163	LYS	2.6
1	B	119	PHE	2.6
1	B	201	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	24	SER	2.6
1	A	314	MET	2.6
1	A	203	ALA	2.6
1	B	282	THR	2.6
1	B	0	HIS	2.5
1	A	310	LEU	2.5
1	B	5	LYS	2.5
1	B	148	LYS	2.5
1	B	188	GLY	2.5
1	B	218	HIS	2.5
1	A	318	ASP	2.5
1	B	129	GLY	2.5
1	B	310	LEU	2.5
1	B	287	SER	2.5
1	B	213	ALA	2.5
1	A	198	ILE	2.4
1	B	198	ILE	2.4
1	B	95	ASP	2.4
1	A	311	PRO	2.4
1	A	306	ASP	2.4
1	B	68	VAL	2.4
1	B	256	ARG	2.4
1	B	140	PRO	2.4
1	B	118	SER	2.4
1	A	158	GLU	2.3
1	B	43	GLU	2.3
1	B	240	PHE	2.3
1	A	309	ILE	2.3
1	A	42	VAL	2.3
1	A	282	THR	2.3
1	B	114	THR	2.3
1	A	196	ARG	2.3
1	A	293	ARG	2.3
1	B	223	ILE	2.3
1	A	302	VAL	2.3
1	B	71	LEU	2.3
1	B	204	LEU	2.3
1	A	102	PHE	2.2
1	B	199	ILE	2.2
1	A	41	VAL	2.2
1	B	106	VAL	2.2
1	A	63	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	243	GLU	2.2
1	A	308	GLY	2.2
1	B	173	ASP	2.2
1	B	312	ASP	2.2
1	A	187	ALA	2.2
1	B	193	GLU	2.2
1	A	143	SER	2.2
1	A	6	GLU	2.1
1	B	109	ILE	2.1
1	A	68	VAL	2.1
1	B	221	ARG	2.1
1	B	200	ILE	2.1
1	A	97	LYS	2.1
1	A	127	LYS	2.1
1	A	46	GLU	2.1
1	A	71	LEU	2.1
1	A	303	TYR	2.1
1	B	306	ASP	2.1
1	B	314	MET	2.1
1	B	66	PRO	2.1
1	A	275	LEU	2.1
1	B	157	LEU	2.1
1	B	251	PHE	2.0
1	B	124	VAL	2.0
1	B	164	LEU	2.0
1	A	1	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](#)

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($\text{\AA}^2$)	Q<0.9
2	MN	A	402	1/1	0.91	0.16	39,39,39,39	1
2	MN	B	402	1/1	0.94	0.21	43,43,43,43	1
2	MN	B	401	1/1	0.99	0.06	28,28,28,28	1
2	MN	A	401	1/1	0.99	0.05	33,33,33,33	1

6.5 Other polymers [i](#)

There are no such residues in this entry.