



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:46 AM UTC

PDB ID : 5IJL / pdb_00005ijl
Title : D-family DNA polymerase - DP2 subunit (catalytic subunit)
Authors : Sauguet, L.; Raia, P.; De Larue, M.
Deposited on : 2016-03-02
Resolution : 2.19 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

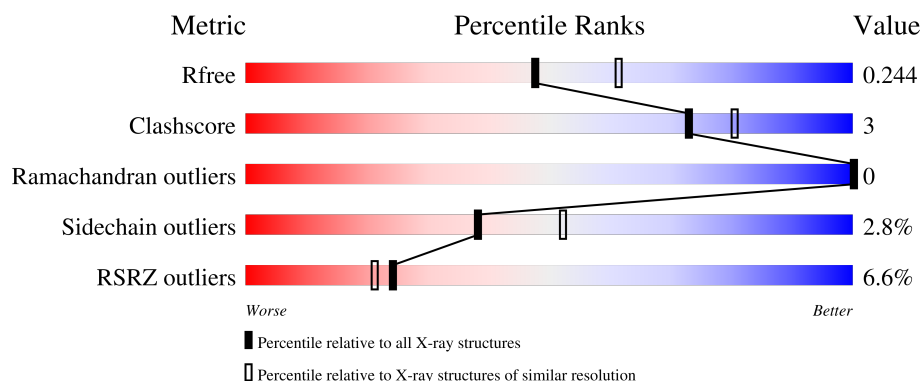
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	1066	6% 78% 10% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7769 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 polymerase II large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	943	7525	4844	1266	1388	27	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q9V2F4
A	-3	THR	-	expression tag	UNP Q9V2F4
A	-2	GLY	-	expression tag	UNP Q9V2F4
A	-1	ASP	-	expression tag	UNP Q9V2F4
A	0	GLY	-	expression tag	UNP Q9V2F4
A	1	SER	-	expression tag	UNP Q9V2F4

- 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		

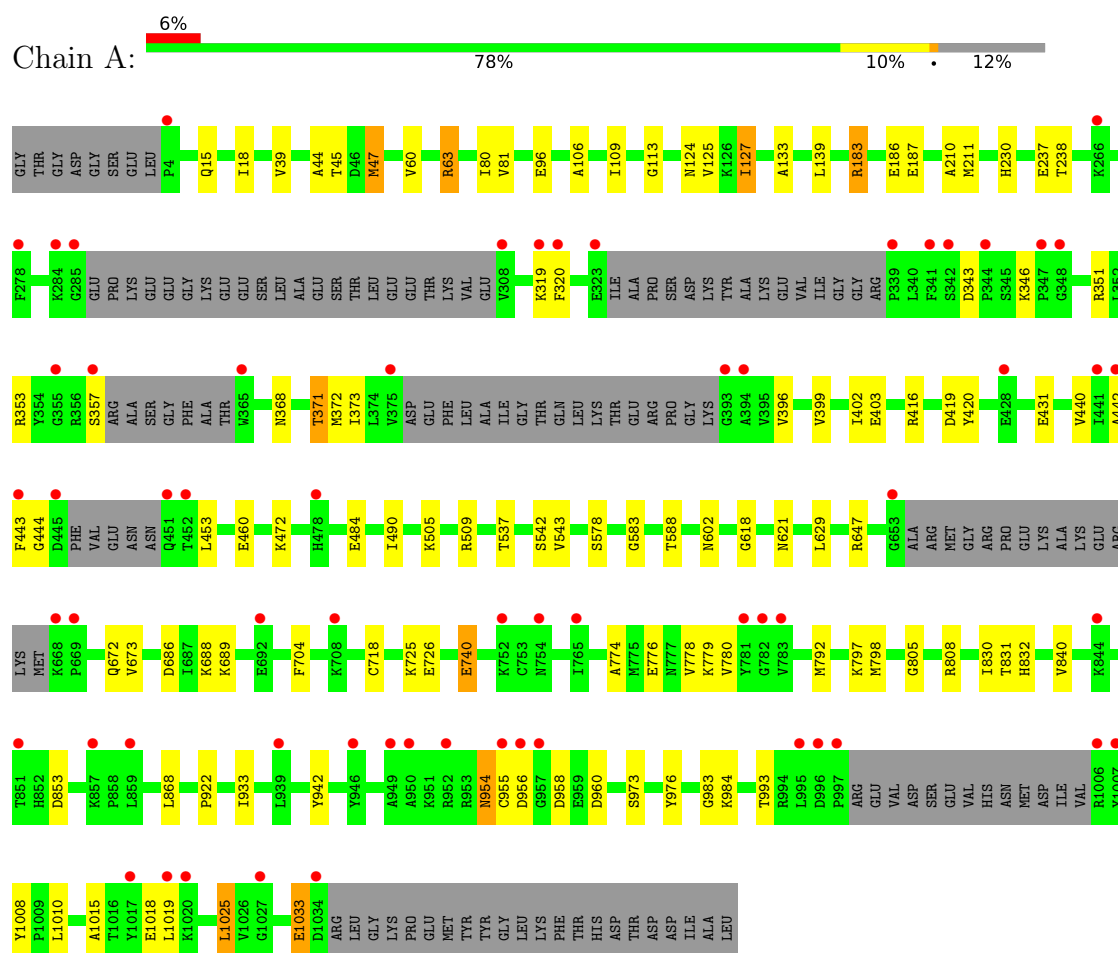
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	242	Total	O	0	0
			242	242		

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: DNA polymerase II large subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.82Å 106.20Å 110.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.80 – 2.19 43.80 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.80-2.19) 99.3 (43.80-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.18Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.199 , 0.235 0.205 , 0.244	Depositor DCC
R_{free} test set	3169 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7769	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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	0.87	0/7695	1.30	38/10408 (0.4%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	955	CYS	N-CA-C	-10.50	101.84	112.97
1	A	955	CYS	CA-C-N	9.67	140.00	121.54
1	A	955	CYS	C-N-CA	9.67	140.00	121.54
1	A	133	ALA	N-CA-C	8.29	128.46	110.80
1	A	320	PHE	CA-CB-CG	7.88	121.68	113.80
1	A	1019	LEU	N-CA-C	6.36	124.35	110.80
1	A	444	GLY	N-CA-C	-6.27	98.32	113.18
1	A	1018	GLU	CA-C-N	6.00	133.00	121.54
1	A	1018	GLU	C-N-CA	6.00	133.00	121.54
1	A	319	LYS	CA-C-N	5.86	128.13	120.28
1	A	319	LYS	C-N-CA	5.86	128.13	120.28
1	A	797	LYS	CA-C-N	5.82	129.43	121.74
1	A	797	LYS	C-N-CA	5.82	129.43	121.74
1	A	210	ALA	CA-C-N	5.79	128.04	120.28
1	A	210	ALA	C-N-CA	5.79	128.04	120.28
1	A	983	GLY	CA-C-N	5.74	127.97	120.28
1	A	983	GLY	C-N-CA	5.74	127.97	120.28
1	A	127	ILE	N-CA-CB	5.68	116.91	110.72
1	A	39	VAL	N-CA-C	-5.60	102.30	109.30
1	A	460	GLU	CA-C-N	5.46	127.60	120.28
1	A	460	GLU	C-N-CA	5.46	127.60	120.28
1	A	60	VAL	N-CA-C	5.45	117.91	111.09
1	A	419	ASP	CA-C-N	5.45	127.90	120.54
1	A	419	ASP	C-N-CA	5.45	127.90	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ALA	CA-C-N	5.45	128.02	120.29
1	A	44	ALA	C-N-CA	5.45	128.02	120.29
1	A	583	GLY	CA-C-N	5.36	128.00	120.28
1	A	583	GLY	C-N-CA	5.36	128.00	120.28
1	A	853	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	542	SER	N-CA-C	-5.31	106.80	113.28
1	A	113	GLY	CA-C-N	5.29	129.01	120.82
1	A	113	GLY	C-N-CA	5.29	129.01	120.82
1	A	1033	GLU	CA-C-N	5.21	131.07	121.70
1	A	1033	GLU	C-N-CA	5.21	131.07	121.70
1	A	444	GLY	CA-C-N	5.13	130.93	121.70
1	A	444	GLY	C-N-CA	5.13	130.93	121.70
1	A	776	GLU	CA-C-N	5.09	127.09	120.28
1	A	776	GLU	C-N-CA	5.09	127.09	120.28

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	7525	0	7562	48	0
2	A	2	0	0	0	0
3	A	242	0	0	3	0
All	All	7769	0	7562	48	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 3.

All (48) 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:183:ARG:NH2	1:A:238:THR:O	2.12	0.81
1:A:357:SER:OG	1:A:442:ALA:HB2	1.85	0.77
1:A:831:THR:HG23	1:A:832:HIS:ND1	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLU:HG3	1:A:127:ILE:HG12	1.74	0.69
1:A:47:MET:HE1	1:A:109:ILE:HG23	1.75	0.69
1:A:183:ARG:NH1	1:A:187:GLU:OE2	2.29	0.65
1:A:186:GLU:OE1	1:A:230:HIS:HD2	1.82	0.63
1:A:830:ILE:HG12	1:A:942:TYR:HB3	1.81	0.63
1:A:373:ILE:HD11	1:A:420:TYR:CD2	2.35	0.61
1:A:954:ASN:C	1:A:956:ASP:H	2.08	0.60
1:A:673:VAL:HB	1:A:805:GLY:HA3	1.84	0.59
1:A:371:THR:HG21	3:A:1237:HOH:O	2.04	0.57
1:A:778:VAL:HG23	1:A:780:VAL:HG22	1.87	0.57
1:A:443:PHE:HB3	1:A:1008:TYR:OH	2.06	0.56
1:A:484:GLU:HG3	1:A:509:ARG:HH21	1.72	0.55
1:A:357:SER:OG	1:A:442:ALA:CB	2.54	0.54
1:A:647:ARG:O	1:A:647:ARG:HG2	2.07	0.54
1:A:351:ARG:HD2	1:A:647:ARG:O	2.09	0.53
1:A:81:VAL:HG23	1:A:106:ALA:HB2	1.91	0.52
1:A:726:GLU:HG2	1:A:740:GLU:HB2	1.92	0.52
1:A:403:GLU:HG2	1:A:416:ARG:HH22	1.73	0.52
1:A:343:ASP:HB3	1:A:346:LYS:HB2	1.92	0.51
1:A:922:PRO:HB3	1:A:984:LYS:HG2	1.91	0.51
1:A:372:MET:HE2	1:A:396:VAL:HG12	1.94	0.49
1:A:63:ARG:HB3	1:A:80:ILE:HD11	1.94	0.47
1:A:211:MET:HE1	3:A:1227:HOH:O	2.15	0.47
1:A:840:VAL:HG21	1:A:933:ILE:O	2.15	0.46
1:A:402:ILE:HD13	1:A:440:VAL:HG23	1.98	0.46
1:A:537:THR:O	1:A:647:ARG:HD2	2.17	0.45
1:A:830:ILE:HG13	1:A:868:LEU:HD22	1.99	0.45
1:A:973:SER:HB3	1:A:976:TYR:CD2	2.52	0.45
1:A:490:ILE:HG21	1:A:505:LYS:HG3	1.98	0.44
1:A:371:THR:CG2	3:A:1237:HOH:O	2.65	0.44
1:A:543:VAL:HG11	1:A:588:THR:HG23	1.99	0.44
1:A:1015:ALA:HB3	1:A:1025:LEU:HD21	1.99	0.44
1:A:353:ARG:O	1:A:440:VAL:HA	2.19	0.43
1:A:673:VAL:HB	1:A:805:GLY:CA	2.48	0.42
1:A:368:ASN:HA	1:A:399:VAL:O	2.19	0.42
1:A:686:ASP:HB3	1:A:689:LYS:HB2	2.01	0.42
1:A:672:GLN:O	1:A:808:ARG:HD2	2.20	0.41
1:A:18:ILE:HD13	1:A:993:THR:HB	2.02	0.41
1:A:125:VAL:CG1	1:A:139:LEU:HD11	2.51	0.41
1:A:125:VAL:HG12	1:A:139:LEU:HD11	2.03	0.41
1:A:578:SER:HA	1:A:602:ASN:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:PHE:HZ	1:A:798:MET:HG3	1.86	0.41
1:A:774:ALA:O	1:A:778:VAL:HG22	2.21	0.41
1:A:618:GLY:O	1:A:621:ASN:HB2	2.20	0.40
1:A:718:CYS:HA	1:A:725:LYS:HD2	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	928/1066 (87%)	902 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	801/907 (88%)	779 (97%)	22 (3%)	39	53

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	45	THR

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Mol	Chain	Res	Type
1	A	47	MET
1	A	63	ARG
1	A	124	ASN
1	A	183	ARG
1	A	237	GLU
1	A	371	THR
1	A	431	GLU
1	A	453	LEU
1	A	472	LYS
1	A	629	LEU
1	A	688	LYS
1	A	740	GLU
1	A	779	LYS
1	A	792	MET
1	A	954	ASN
1	A	958	ASP
1	A	960	ASP
1	A	1010	LEU
1	A	1025	LEU
1	A	1033	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	180	HIS
1	A	201	HIS
1	A	213	ASN
1	A	230	HIS
1	A	255	GLN
1	A	421	ASN
1	A	557	ASN
1	A	565	ASN
1	A	602	ASN
1	A	639	ASN
1	A	711	HIS
1	A	720	ASN
1	A	742	GLN
1	A	747	ASN
1	A	852	HIS
1	A	923	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	943/1066 (88%)	0.34	62 (6%)	24 21	31, 48, 83, 119	1 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	320	PHE	5.1
1	A	308	VAL	4.9
1	A	1019	LEU	4.5
1	A	957	GLY	4.5
1	A	357	SER	4.4
1	A	445	ASP	4.4
1	A	285	GLY	4.3
1	A	946	TYR	3.9
1	A	323	GLU	3.9
1	A	375	VAL	3.9
1	A	997	PRO	3.8
1	A	1020	LYS	3.6
1	A	4	PRO	3.3
1	A	365	TRP	3.2
1	A	996	ASP	3.2
1	A	668	LYS	3.2
1	A	347	PRO	3.1
1	A	341	PHE	3.1
1	A	851	THR	3.0
1	A	394	ALA	3.0
1	A	955	CYS	3.0
1	A	781	TYR	3.0
1	A	956	ASP	2.9
1	A	339	PRO	2.9
1	A	708	LYS	2.8
1	A	393	GLY	2.8
1	A	950	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	441	ILE	2.7
1	A	452	THR	2.7
1	A	949	ALA	2.7
1	A	653	GLY	2.7
1	A	669	PRO	2.6
1	A	428	GLU	2.6
1	A	1034	ASP	2.6
1	A	355	GLY	2.6
1	A	752	LYS	2.6
1	A	478[A]	HIS	2.5
1	A	266	LYS	2.5
1	A	844	LYS	2.5
1	A	939	LEU	2.5
1	A	348	GLY	2.5
1	A	442	ALA	2.4
1	A	443	PHE	2.4
1	A	1027	GLY	2.4
1	A	754	ASN	2.4
1	A	952	ARG	2.4
1	A	342	SER	2.4
1	A	451	GLN	2.3
1	A	1007	TYR	2.3
1	A	692	GLU	2.3
1	A	278	PHE	2.3
1	A	284	LYS	2.3
1	A	319	LYS	2.2
1	A	1017	TYR	2.2
1	A	783	VAL	2.2
1	A	857	LYS	2.1
1	A	765	ILE	2.1
1	A	782	GLY	2.1
1	A	1006	ARG	2.1
1	A	344	PRO	2.1
1	A	859	LEU	2.0
1	A	995	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	ZN	A	1102	1/1	0.98	0.05	99,99,99,99	0
2	ZN	A	1101	1/1	0.99	0.03	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.