



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:36 AM UTC

PDB ID : 9BOR / pdb_00009bor
Title : IkappaBzeta ankyrin repeat domain:NF-kappaB p50 homodimer complex at 2.0 Angstrom resolution
Authors : Rogers, W.E.; Zhu, N.; Huxford, T.
Deposited on : 2024-05-05
Resolution : 2.00 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

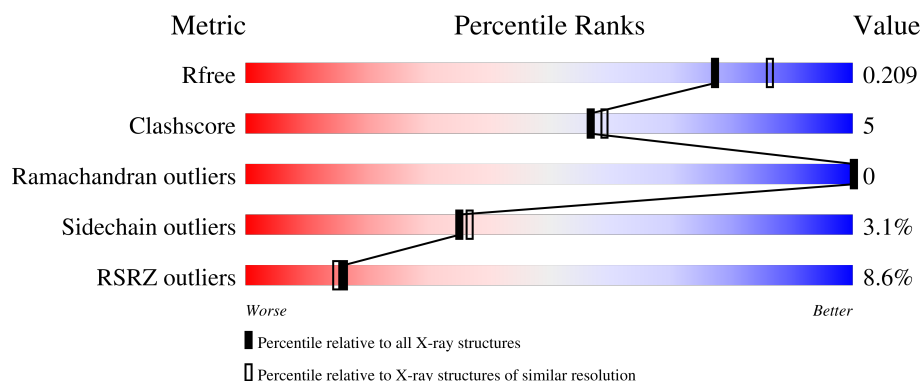
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	315	11% 80% 12% 6%
2	B	132	2% 85% 6% 9%
2	C	132	6% 73% 6% 18%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4475 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.

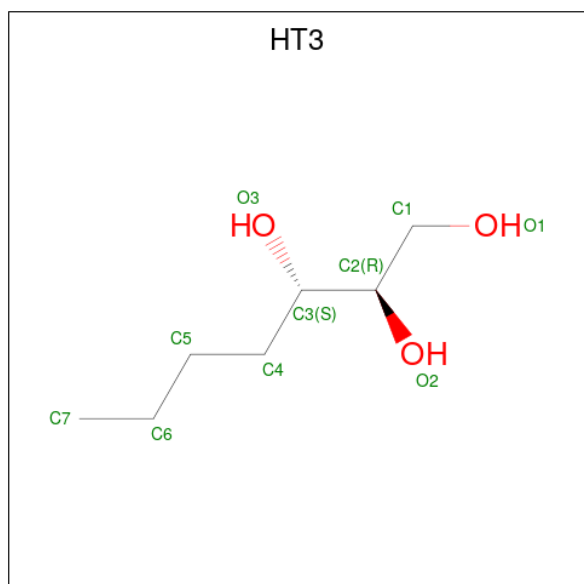
- Molecule 1 is a protein called NF-kappa-B inhibitor zeta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2282	1425	421	427	9			

- Molecule 2 is a protein called Nuclear factor NF-kappa-B p50 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	S	0	0	0
			989	632	168	185	4			
2	C	108	Total	C	N	O	S	0	0	0
			876	563	145	165	3			

- Molecule 3 is (2R,3S)-heptane-1,2,3-triol (CCD ID: HT3) (formula: C₇H₁₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	7	3		

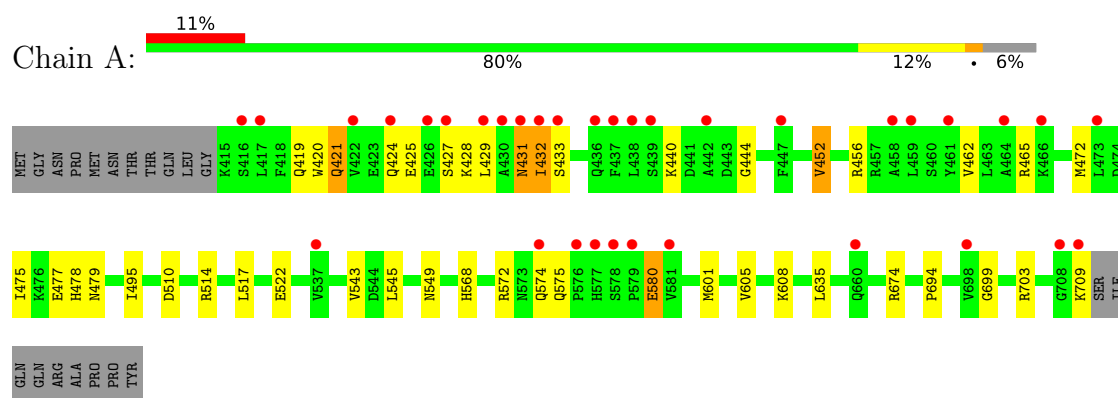
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	134	Total 134	O 134	0	0
4	B	97	Total 97	O 97	0	0
4	C	87	Total 87	O 87	0	0

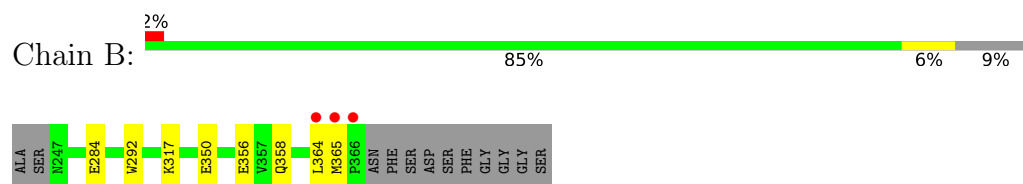
3 Residue-property plots [i](#)

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.

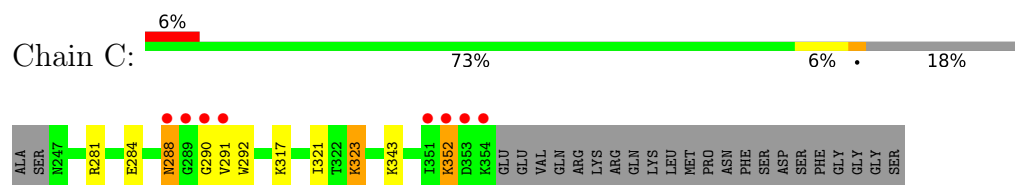
- Molecule 1: NF-kappa-B inhibitor zeta



- Molecule 2: Nuclear factor NF-kappa-B p50 subunit



- Molecule 2: Nuclear factor NF-kappa-B p50 subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.41Å 58.93Å 108.81Å 90.00° 99.15° 90.00°	Depositor
Resolution (Å)	43.31 – 2.00 43.31 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (43.31-2.00) 98.9 (43.31-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.181 , 0.208 0.184 , 0.209	Depositor DCC
R_{free} test set	2186 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4475	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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: HT3

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	0.35	0/2318	0.75	6/3141 (0.2%)
2	B	0.35	0/1010	0.72	0/1358
2	C	0.36	0/896	0.72	0/1209
All	All	0.35	0/4224	0.74	6/5708 (0.1%)

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	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	ILE	N-CA-C	8.11	118.87	110.36
1	A	432	ILE	CA-C-N	5.69	131.93	121.70
1	A	432	ILE	C-N-CA	5.69	131.93	121.70
1	A	432	ILE	CA-C-O	-5.56	115.49	121.27
1	A	575	GLN	CA-C-N	5.39	124.58	118.97
1	A	575	GLN	C-N-CA	5.39	124.58	118.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	431	ASN	Peptide

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	2282	0	2292	27	0
2	B	989	0	986	4	0
2	C	876	0	857	8	0
3	B	10	0	16	1	0
4	A	134	0	0	6	2
4	B	97	0	0	1	1
4	C	87	0	0	2	1
All	All	4475	0	4151	38	2

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 5.

All (38) 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:432:ILE:HG23	1:A:433:SER:HA	1.48	0.93
2:B:350:GLU:OE1	4:B:501:HOH:O	2.04	0.73
1:A:572:ARG:O	1:A:574:GLN:NE2	2.22	0.72
1:A:477:GLU:HG3	1:A:479:ASN:H	1.56	0.71
1:A:465:ARG:O	4:A:802:HOH:O	2.11	0.68
1:A:472:MET:HE3	1:A:475:ILE:HD11	1.79	0.65
1:A:425:GLU:HA	1:A:428:LYS:HD2	1.80	0.64
1:A:703:ARG:NH2	4:A:804:HOH:O	2.29	0.63
2:C:343:LYS:NZ	4:C:401:HOH:O	2.32	0.61
1:A:674:ARG:NE	4:A:801:HOH:O	2.07	0.61
1:A:522:GLU:OE1	4:A:803:HOH:O	2.15	0.59
2:C:284:GLU:HG2	4:C:454:HOH:O	2.02	0.58
1:A:608:LYS:NZ	4:A:806:HOH:O	2.32	0.57
2:B:292:TRP:CD1	2:B:317:LYS:HB3	2.40	0.56
2:C:288:ASN:HD21	2:C:290:GLY:C	2.13	0.56
1:A:549:ASN:HB2	4:A:835:HOH:O	2.09	0.52
1:A:440:LYS:NZ	1:A:444:GLY:O	2.33	0.51
2:C:281:ARG:NH2	2:C:291:VAL:HG11	2.27	0.50
2:B:284:GLU:HG3	3:B:401:HT3:H4A	1.93	0.50
1:A:421:GLN:OE1	1:A:425:GLU:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:GLN:O	1:A:427:SER:HB3	2.13	0.49
1:A:517:LEU:HD11	1:A:543:VAL:HG12	1.93	0.48
1:A:420:TRP:O	1:A:424:GLN:HB2	2.14	0.48
2:C:292:TRP:CD1	2:C:317:LYS:HB3	2.50	0.47
1:A:452:VAL:HG22	1:A:495:ILE:HG21	1.96	0.46
1:A:580:GLU:H	1:A:580:GLU:HG2	1.53	0.45
1:A:478:HIS:NE2	2:B:356:GLU:OE2	2.49	0.43
1:A:425:GLU:O	1:A:428:LYS:N	2.45	0.42
1:A:510:ASP:OD2	1:A:514:ARG:HD3	2.19	0.42
2:C:352:LYS:HE2	2:C:352:LYS:HB2	1.84	0.41
2:C:321:ILE:HD12	2:C:323:LYS:O	2.20	0.41
2:C:288:ASN:ND2	2:C:290:GLY:H	2.18	0.41
1:A:568:HIS:O	1:A:572:ARG:HG3	2.20	0.41
1:A:425:GLU:HB3	1:A:462:VAL:HG21	2.02	0.41
1:A:545:LEU:HD21	1:A:601:MET:HE2	2.03	0.41
1:A:572:ARG:HE	1:A:572:ARG:HB3	1.59	0.41
1:A:694:PRO:O	1:A:699:GLY:HA3	2.21	0.40
1:A:605:VAL:HG21	1:A:635:LEU:CD1	2.51	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:927:HOH:O	4:B:588:HOH:O[1_655]	2.01	0.19
4:A:873:HOH:O	4:C:447:HOH:O[2_556]	2.19	0.01

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	293/315 (93%)	282 (96%)	11 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	118/132 (89%)	117 (99%)	1 (1%)	0	100	100
2	C	106/132 (80%)	101 (95%)	5 (5%)	0	100	100
All	All	517/579 (89%)	500 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	244/263 (93%)	236 (97%)	8 (3%)	33	34
2	B	109/118 (92%)	106 (97%)	3 (3%)	38	41
2	C	95/118 (80%)	92 (97%)	3 (3%)	34	35
All	All	448/499 (90%)	434 (97%)	14 (3%)	35	37

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

Mol	Chain	Res	Type
1	A	419	GLN
1	A	421	GLN
1	A	429	LEU
1	A	431	ASN
1	A	452	VAL
1	A	456	ARG
1	A	580	GLU
1	A	709	LYS
2	B	358	GLN
2	B	364	LEU
2	B	365	MET
2	C	288	ASN
2	C	323	LYS
2	C	352	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	471	HIS
1	A	577	HIS
2	C	288	ASN

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	HT3	B	401	-	9,9,9	0.82	0	10,10,10	1.37	2 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HT3	B	401	-	-	5/10/10/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	401	HT3	C5-C4-C3	-2.58	109.88	114.11
3	B	401	HT3	C1-C2-C3	-2.40	108.11	113.00

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	HT3	O1-C1-C2-O2
3	B	401	HT3	O1-C1-C2-C3
3	B	401	HT3	O2-C2-C3-C4
3	B	401	HT3	O2-C2-C3-O3
3	B	401	HT3	C4-C5-C6-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	HT3	1	0

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	295/315 (93%)	0.70	34 (11%) 9 8	25, 44, 93, 104	0
2	B	120/132 (90%)	-0.08	3 (2%) 58 58	22, 30, 71, 97	0
2	C	108/132 (81%)	0.12	8 (7%) 20 19	20, 32, 94, 111	0
All	All	523/579 (90%)	0.40	45 (8%) 16 15	20, 38, 92, 111	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	290	GLY	7.0
1	A	429	LEU	6.3
2	C	289	GLY	5.8
1	A	432	ILE	5.4
1	A	430	ALA	5.2
2	C	291	VAL	4.8
2	B	366	PRO	4.6
1	A	576	PRO	3.7
1	A	438	LEU	3.6
1	A	660	GLN	3.5
1	A	447	PHE	3.5
2	C	288	ASN	3.3
1	A	427	SER	3.3
1	A	437	PHE	3.2
1	A	464	ALA	3.1
2	B	364	LEU	3.0
2	C	354	LYS	2.9
1	A	433	SER	2.9
1	A	579	PRO	2.9
2	C	353	ASP	2.9
1	A	422	VAL	2.8
1	A	578	SER	2.8
1	A	577	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	442	ALA	2.8
1	A	581	VAL	2.8
1	A	436	GLN	2.7
2	B	365	MET	2.6
1	A	417	LEU	2.6
1	A	708	GLY	2.5
2	C	352	LYS	2.5
1	A	466	LYS	2.5
1	A	424	GLN	2.5
1	A	416	SER	2.4
1	A	537	VAL	2.4
1	A	459	LEU	2.4
2	C	351	ILE	2.3
1	A	458	ALA	2.3
1	A	431	ASN	2.3
1	A	461	TYR	2.2
1	A	439	SER	2.2
1	A	473	LEU	2.1
1	A	709	LYS	2.1
1	A	426	GLU	2.1
1	A	574	GLN	2.1
1	A	698	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
3	HT3	B	401	10/10	0.79	0.18	32,41,46,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.