



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:57 AM UTC

PDB ID : 4F01 / pdb_00004f01
Title : Crystal structure of an artificial dimeric DnaK complex
Authors : Zahn, M.; Straeter, N.
Deposited on : 2012-05-03
Resolution : 1.40 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

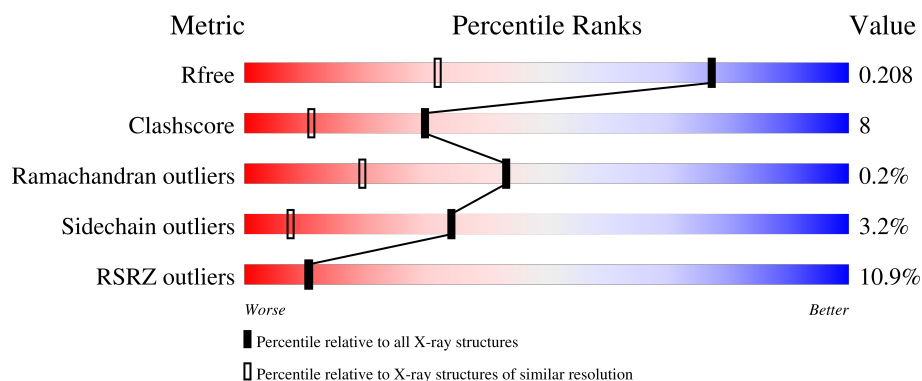
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	241	2% 84% 5% 10%
1	B	241	19% 76% 15% 5%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3846 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 Chaperone protein DnaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	8	0
			1690	1041	294	346	9			
1	B	230	Total	C	N	O	S	0	3	0
			1782	1094	323	356	9			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	367	MET	-	expression tag	UNP P0A6Y8
A	368	GLY	-	expression tag	UNP P0A6Y8
A	369	HIS	-	expression tag	UNP P0A6Y8
A	370	HIS	-	expression tag	UNP P0A6Y8
A	371	HIS	-	expression tag	UNP P0A6Y8
A	372	HIS	-	expression tag	UNP P0A6Y8
A	373	HIS	-	expression tag	UNP P0A6Y8
A	374	HIS	-	expression tag	UNP P0A6Y8
A	375	HIS	-	expression tag	UNP P0A6Y8
A	376	HIS	-	expression tag	UNP P0A6Y8
A	377	HIS	-	expression tag	UNP P0A6Y8
A	378	HIS	-	expression tag	UNP P0A6Y8
A	379	SER	-	expression tag	UNP P0A6Y8
A	380	SER	-	expression tag	UNP P0A6Y8
A	381	GLY	-	expression tag	UNP P0A6Y8
A	382	HIS	-	expression tag	UNP P0A6Y8
A	383	ILE	-	expression tag	UNP P0A6Y8
A	384	GLU	-	expression tag	UNP P0A6Y8
A	385	GLY	-	expression tag	UNP P0A6Y8
A	386	ARG	-	expression tag	UNP P0A6Y8
A	387	HIS	-	expression tag	UNP P0A6Y8
A	388	MET	-	expression tag	UNP P0A6Y8
B	367	MET	-	expression tag	UNP P0A6Y8
B	368	GLY	-	expression tag	UNP P0A6Y8
B	369	HIS	-	expression tag	UNP P0A6Y8

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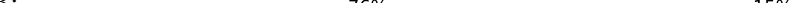
Chain	Residue	Modelled	Actual	Comment	Reference
B	370	HIS	-	expression tag	UNP P0A6Y8
B	371	HIS	-	expression tag	UNP P0A6Y8
B	372	HIS	-	expression tag	UNP P0A6Y8
B	373	HIS	-	expression tag	UNP P0A6Y8
B	374	HIS	-	expression tag	UNP P0A6Y8
B	375	HIS	-	expression tag	UNP P0A6Y8
B	376	HIS	-	expression tag	UNP P0A6Y8
B	377	HIS	-	expression tag	UNP P0A6Y8
B	378	HIS	-	expression tag	UNP P0A6Y8
B	379	SER	-	expression tag	UNP P0A6Y8
B	380	SER	-	expression tag	UNP P0A6Y8
B	381	GLY	-	expression tag	UNP P0A6Y8
B	382	HIS	-	expression tag	UNP P0A6Y8
B	383	ILE	-	expression tag	UNP P0A6Y8
B	384	GLU	-	expression tag	UNP P0A6Y8
B	385	GLY	-	expression tag	UNP P0A6Y8
B	386	ARG	-	expression tag	UNP P0A6Y8
B	387	HIS	-	expression tag	UNP P0A6Y8
B	388	MET	-	expression tag	UNP P0A6Y8

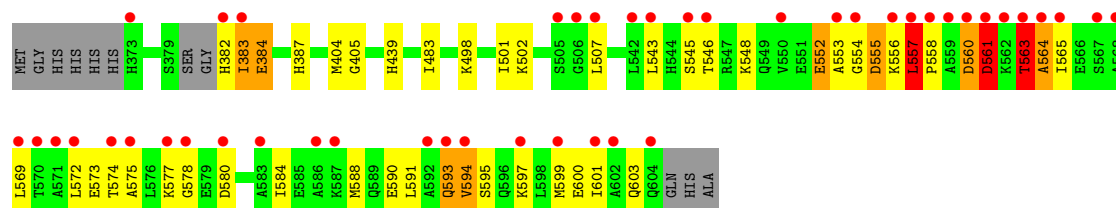
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	255	Total O 255 255	0	0
2	B	119	Total O 119 119	0	0

- Molecule 1: Chaperone protein DnaK



Chain B:  19% 76% 15% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.11Å 61.38Å 69.19Å 90.00° 103.39° 90.00°	Depositor
Resolution (Å)	25.00 – 1.40 25.00 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (25.00-1.40) 98.5 (25.00-1.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 1.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.162 , 0.213 0.160 , 0.208	Depositor DCC
R_{free} test set	1939 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3846	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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

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	1.32	7/1729 (0.4%)	1.16	1/2326 (0.0%)
1	B	1.37	9/1812 (0.5%)	1.20	8/2438 (0.3%)
All	All	1.34	16/3541 (0.5%)	1.18	9/4764 (0.2%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	564	ALA	C-O	7.01	1.32	1.23
1	B	439	HIS	ND1-CE1	6.53	1.39	1.32
1	A	422	HIS	CE1-NE2	6.33	1.38	1.32
1	B	384	GLU	C-O	-6.29	1.16	1.24
1	B	501	ILE	N-CA	6.00	1.53	1.46
1	A	520[A]	GLU	C-O	-5.90	1.16	1.24
1	A	520[B]	GLU	C-O	-5.90	1.16	1.24
1	A	400	GLY	N-CA	5.75	1.52	1.45
1	A	435	ALA	N-CA	5.70	1.53	1.45
1	B	501	ILE	CA-C	5.62	1.59	1.52
1	B	560	ASP	CG-OD1	5.51	1.35	1.25
1	B	563	THR	C-N	5.47	1.41	1.33
1	A	523	ALA	C-O	5.16	1.30	1.24
1	A	551	GLU	C-O	5.13	1.30	1.24
1	B	593	GLN	CD-OE1	5.13	1.33	1.23
1	B	563	THR	C-O	5.04	1.30	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	383	ILE	N-CA-C	6.85	116.97	110.53
1	B	383	ILE	CA-C-N	-6.71	112.88	122.94
1	B	383	ILE	C-N-CA	-6.71	112.88	122.94
1	B	580	ASP	N-CA-C	5.92	118.77	107.75
1	B	561	ASP	N-CA-C	-5.67	104.72	111.69
1	A	534	GLN	CA-CB-CG	5.28	124.67	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	557	LEU	CA-C-N	5.24	126.39	119.84
1	B	557	LEU	C-N-CA	5.24	126.39	119.84
1	B	578	GLY	N-CA-C	5.23	121.14	112.66

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	1690	0	1722	22	0
1	B	1782	0	1782	44	0
2	A	255	0	0	5	0
2	B	119	0	0	0	0
All	All	3846	0	3504	59	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 8.

All (59) 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:404[B]:MET:HA	1:A:404[B]:MET:CE	1.63	1.29
1:A:404[B]:MET:HA	1:A:404[B]:MET:HE2	1.22	1.16
1:B:483:ILE:HD12	1:B:502:LYS:HG2	1.32	1.12
1:A:404[B]:MET:HE1	1:B:387:HIS:CG	1.95	1.01
1:A:404[B]:MET:CE	1:A:404[B]:MET:CA	2.35	0.97
1:A:404[B]:MET:HA	1:A:404[B]:MET:HE3	1.46	0.96
1:B:560:ASP:O	1:B:563:THR:HG22	1.67	0.94
1:A:404[B]:MET:CA	1:A:404[B]:MET:HE3	1.96	0.94
1:B:558:PRO:HD2	1:B:597:LYS:HE3	1.50	0.92
1:B:404[B]:MET:HE3	1:B:405:GLY:H	1.36	0.91
1:B:543:LEU:HD21	1:B:573:GLU:HG2	1.53	0.90
1:B:483:ILE:CD1	1:B:502:LYS:HG2	2.01	0.90
1:A:404[B]:MET:CE	1:B:387:HIS:HB3	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404[B]:MET:HE1	1:B:387:HIS:HB3	1.58	0.84
1:B:600:GLU:O	1:B:603:GLN:HG2	1.78	0.83
1:B:483:ILE:HD12	1:B:502:LYS:CG	2.07	0.83
1:A:404[B]:MET:HE1	1:B:387:HIS:CB	2.09	0.81
1:A:404[B]:MET:HE1	1:B:387:HIS:ND1	2.00	0.77
1:B:558:PRO:CD	1:B:597:LYS:HE3	2.16	0.75
1:A:404[B]:MET:HE2	1:A:404[B]:MET:CA	2.07	0.74
1:B:546:THR:CG2	1:B:569:LEU:HD21	2.24	0.67
1:B:595:SER:O	1:B:599:MET:HG3	1.94	0.66
1:B:404[B]:MET:HE3	1:B:405:GLY:N	2.09	0.65
1:B:543:LEU:CD2	1:B:573:GLU:HG2	2.24	0.65
1:B:553:ALA:HB1	1:B:601:ILE:CG2	2.29	0.63
1:B:404[B]:MET:CE	1:B:405:GLY:H	2.09	0.63
1:A:520[A]:GLU:HG3	2:A:786:HOH:O	2.00	0.60
1:B:554:GLY:O	1:B:556:LYS:N	2.37	0.58
1:B:560:ASP:HA	1:B:563:THR:HB	1.85	0.57
1:B:546:THR:HG21	1:B:569:LEU:HD21	1.85	0.57
1:B:553:ALA:HB1	1:B:601:ILE:HG21	1.86	0.57
1:B:554:GLY:O	1:B:555:ASP:C	2.48	0.56
1:B:572:LEU:HD12	1:B:572:LEU:O	2.07	0.54
1:B:557:LEU:HD11	1:B:601:ILE:HG13	1.90	0.54
1:B:564:ALA:O	1:B:594:VAL:HG11	2.10	0.52
1:B:557:LEU:CD1	1:B:601:ILE:HG13	2.39	0.52
1:B:404[B]:MET:HE3	1:B:404[B]:MET:HA	1.92	0.51
1:A:534:GLN:HG3	2:A:872:HOH:O	2.10	0.49
1:B:553:ALA:HB1	1:B:601:ILE:HG22	1.95	0.49
1:B:383:ILE:HG23	1:B:384:GLU:N	2.28	0.48
1:B:548:LYS:O	1:B:552:GLU:HB3	2.15	0.47
1:A:404[B]:MET:HE3	1:B:387:HIS:HB3	1.92	0.47
1:A:404[B]:MET:CE	1:B:387:HIS:CB	2.79	0.45
1:A:593:GLN:O	1:A:596:GLN:HB2	2.16	0.44
1:B:483:ILE:HD13	1:B:483:ILE:N	2.31	0.44
1:A:534:GLN:HG2	2:A:861:HOH:O	2.17	0.44
1:B:588:MET:HE2	1:B:588:MET:HB3	1.90	0.43
1:B:546:THR:HG21	1:B:591:LEU:HD11	2.01	0.43
1:A:539:GLY:HA3	1:A:576:LEU:HD21	2.00	0.43
1:A:404[B]:MET:HE3	1:A:404[B]:MET:HB2	1.84	0.42
1:B:404[B]:MET:CE	1:B:405:GLY:N	2.78	0.42
1:A:562:LYS:HE3	2:A:926:HOH:O	2.19	0.42
1:B:561:ASP:OD1	1:B:565:ILE:CD1	2.68	0.42
1:B:558:PRO:HB2	1:B:561:ASP:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:ALA:HB1	1:B:584:ILE:HA	2.03	0.41
1:B:546:THR:HG22	1:B:569:LEU:HD11	2.03	0.41
1:A:404[B]:MET:HE2	2:A:866:HOH:O	2.19	0.41
1:A:534:GLN:O	1:A:538:GLN:HG3	2.21	0.40
1:B:590:GLU:O	1:B:593:GLN:HB2	2.21	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	224/241 (93%)	220 (98%)	4 (2%)	0	100	100
1	B	229/241 (95%)	222 (97%)	6 (3%)	1 (0%)	30	10
All	All	453/482 (94%)	442 (98%)	10 (2%)	1 (0%)	43	19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	555	ASP

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/200 (94%)	187 (100%)	1 (0%)	81	61
1	B	195/200 (98%)	184 (94%)	11 (6%)	19	2
All	All	383/400 (96%)	371 (97%)	12 (3%)	34	8

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	556	LYS
1	B	382	HIS
1	B	498	LYS
1	B	507	LEU
1	B	545	SER
1	B	552	GLU
1	B	557	LEU
1	B	561	ASP
1	B	563	THR
1	B	574	THR
1	B	577	LYS
1	B	594	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	463	ASN
1	B	424	GLN
1	B	432	ASN
1	B	497	GLN

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](#)

There are no ligands in this entry.

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	218/241 (90%)	-0.18	4 (1%) 67 71	8, 18, 43, 73	8 (3%)
1	B	230/241 (95%)	0.87	45 (19%) 3 3	7, 31, 94, 144	3 (1%)
All	All	448/482 (92%)	0.36	49 (10%) 10 11	7, 23, 77, 144	11 (2%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	563	THR	9.0
1	B	564	ALA	8.2
1	B	586	ALA	6.9
1	B	561	ASP	6.7
1	B	545	SER	6.2
1	B	559	ALA	6.0
1	B	574	THR	5.8
1	B	568	ALA	5.3
1	B	383	ILE	5.0
1	B	553	ALA	4.7
1	B	571	ALA	4.5
1	B	557	LEU	4.5
1	B	570	THR	4.4
1	A	602	ALA	4.2
1	B	560	ASP	4.0
1	B	558	PRO	3.8
1	B	601	ILE	3.8
1	B	554	GLY	3.7
1	B	565	ILE	3.3
1	B	550	VAL	3.3
1	B	594	VAL	3.3
1	B	575	ALA	3.2
1	B	506	GLY	3.2
1	B	569	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	592	ALA	3.1
1	B	599	MET	3.1
1	B	382	HIS	3.1
1	B	583	ALA	3.0
1	B	546	THR	2.9
1	B	505	SER	2.9
1	B	602	ALA	2.8
1	B	542	LEU	2.8
1	B	562	LYS	2.8
1	B	556	LYS	2.6
1	B	373	HIS	2.6
1	A	582	ALA	2.5
1	B	597	LYS	2.5
1	B	543	LEU	2.4
1	A	583	ALA	2.4
1	B	587	LYS	2.4
1	B	567	SER	2.3
1	B	572	LEU	2.3
1	B	578	GLY	2.2
1	B	604	GLN	2.1
1	B	577	LYS	2.1
1	B	593	GLN	2.1
1	A	540	ASP	2.1
1	B	580	ASP	2.0
1	B	507	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.