



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:31 AM UTC

PDB ID : 3EAR / pdb_00003ear
Title : Novel dimerization motif in the DEAD box RNA helicase Hera: form 1, partial dimer
Authors : Klostermeier, D.; Rudolph, M.G.
Deposited on : 2008-08-26
Resolution : 2.30 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
Xtrriage (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

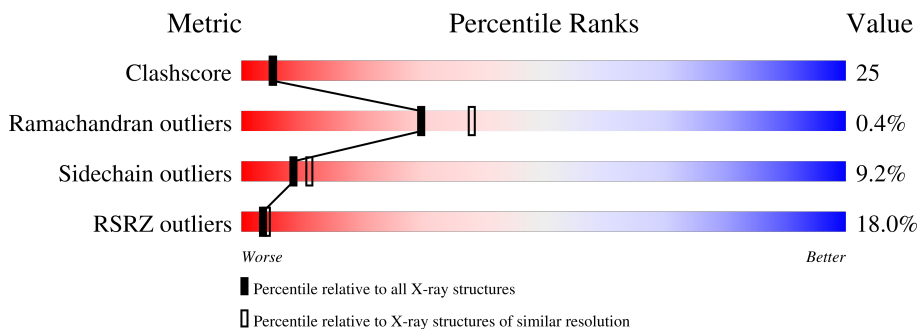
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	212	
1	B	212	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2081 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 Hera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	206	1640	1030	316	293	1	0	0	0
1	B	50	412	268	74	70		0	0	0

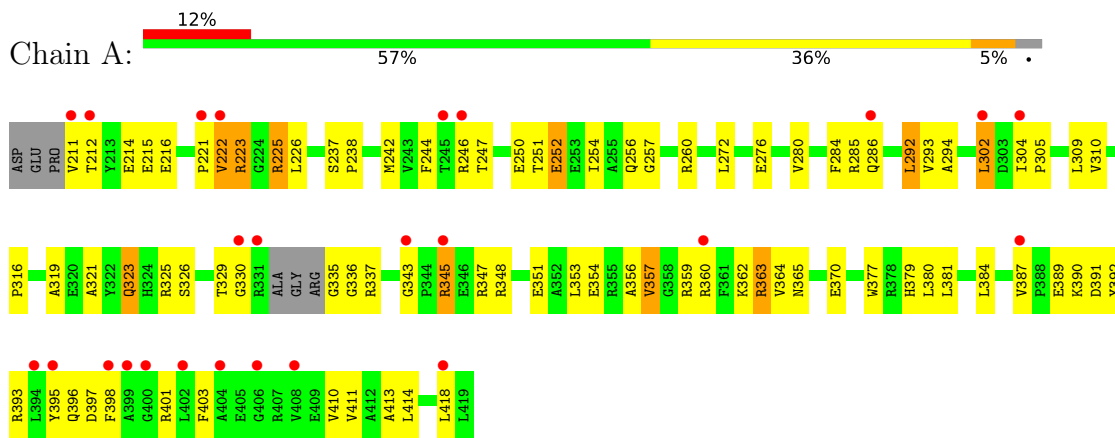
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	27	Total	O	0	0
			27	27		
2	B	2	Total	O	0	0
			2	2		

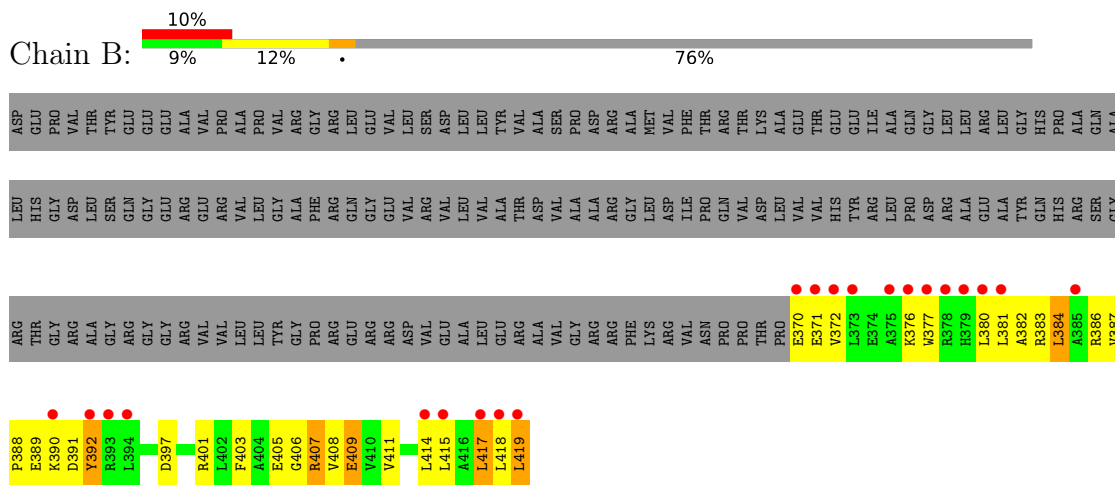
3 Residue-property plots i

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: Hera



- Molecule 1: Hera



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	41.56Å 67.72Å 183.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.93 – 2.30 45.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.93-2.30) 99.4 (45.93-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.231 , 0.255 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtrriage
Anisotropy	0.554	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2081	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.30% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.45	0/1668	0.84	3/2255 (0.1%)
1	B	0.28	0/419	0.73	0/564
All	All	0.42	0/2087	0.82	3/2819 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	GLY	CA-C-N	5.86	125.06	118.97
1	A	343	GLY	C-N-CA	5.86	125.06	118.97
1	A	304	ILE	CB-CA-C	-5.34	104.99	110.71

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	1640	0	1671	78	0
1	B	412	0	427	34	0
2	A	27	0	0	2	0
2	B	2	0	0	0	0
All	All	2081	0	2098	102	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 25.

All (102) 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:392:TYR:HE1	1:A:396:GLN:HE21	1.29	0.80
1:A:389:GLU:HG2	1:A:393:ARG:HD2	1.64	0.80
1:A:389:GLU:O	1:A:393:ARG:HG3	1.85	0.76
1:B:370:GLU:HG2	1:B:371:GLU:H	1.52	0.74
1:B:389:GLU:HA	1:B:392:TYR:CE2	2.23	0.74
1:A:316:PRO:HD2	1:A:353:LEU:HD11	1.69	0.74
1:A:347:ARG:O	1:A:351:GLU:HG3	1.90	0.70
1:A:221:PRO:CB	1:A:223:ARG:HE	2.07	0.68
1:A:242:MET:HE3	1:A:294:ALA:HB3	1.76	0.67
1:A:403:PHE:HE2	1:B:411:VAL:HG21	1.59	0.67
1:A:395:TYR:HB3	1:B:415:LEU:HD11	1.78	0.64
1:A:242:MET:HE2	1:A:244:PHE:CZ	2.34	0.63
1:A:272:LEU:HD22	1:A:276:GLU:HB3	1.81	0.63
1:A:360:ARG:HD3	2:A:29:HOH:O	1.97	0.63
1:A:221:PRO:HB3	1:A:223:ARG:HE	1.62	0.62
1:A:237:SER:HG	1:A:379:HIS:HE2	1.47	0.61
1:A:387:VAL:HG12	1:A:392:TYR:HD2	1.64	0.61
1:A:242:MET:HE2	1:A:244:PHE:CE2	2.36	0.61
1:B:380:LEU:HD22	1:B:419:LEU:HD11	1.82	0.61
1:B:409:GLU:H	1:B:409:GLU:CD	2.10	0.60
1:A:222:VAL:HA	1:A:225:ARG:HD3	1.82	0.59
1:B:388:PRO:C	1:B:390:LYS:H	2.10	0.59
1:B:370:GLU:HG2	1:B:371:GLU:N	2.16	0.59
1:B:372:VAL:O	1:B:376:LYS:HE2	2.04	0.58
1:A:403:PHE:HE1	1:B:406:GLY:HA2	1.70	0.57
1:A:211:VAL:HG21	1:A:359:ARG:CZ	2.35	0.56
1:A:418:LEU:HB2	1:B:418:LEU:HD21	1.86	0.56
1:A:247:THR:OG1	1:A:250:GLU:HG3	2.06	0.55
1:A:223:ARG:HH11	1:A:223:ARG:HB3	1.71	0.55
1:A:380:LEU:O	1:A:384:LEU:HG	2.07	0.55
1:A:215:GLU:OE1	1:A:359:ARG:HD2	2.07	0.54
1:A:252:GLU:O	1:A:256:GLN:HG2	2.06	0.54
1:A:302:LEU:HD12	1:A:302:LEU:N	2.23	0.54
1:B:381:LEU:HA	1:B:384:LEU:HB2	1.89	0.54
1:A:212:THR:O	1:A:335:GLY:HA3	2.08	0.53
1:B:406:GLY:O	1:B:408:VAL:HG23	2.08	0.53
1:A:397:ASP:O	1:A:401:ARG:HG3	2.09	0.53
1:A:403:PHE:CE2	1:B:411:VAL:HG21	2.43	0.52
1:A:221:PRO:HB2	1:A:223:ARG:HE	1.74	0.52
1:A:221:PRO:HB2	1:A:223:ARG:NE	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:HD11	1:B:417:LEU:HD12	1.91	0.52
1:A:302:LEU:HD12	1:A:302:LEU:H	1.73	0.52
1:A:411:VAL:HA	1:A:414:LEU:HD12	1.91	0.52
1:A:330:GLY:HA3	1:A:335:GLY:HA2	1.92	0.51
1:A:285:ARG:HG3	1:A:305:PRO:HG3	1.93	0.51
1:B:382:ALA:O	1:B:386:ARG:HG3	2.10	0.51
1:B:388:PRO:HG2	1:B:391:ASP:OD1	2.11	0.51
1:A:326:SER:O	1:A:329:THR:HG22	2.10	0.50
1:B:397:ASP:O	1:B:401:ARG:HG3	2.12	0.50
1:A:285:ARG:CG	1:A:305:PRO:HG3	2.42	0.49
1:A:309:LEU:HD12	1:A:337:ARG:O	2.12	0.49
1:A:216:GLU:OE1	1:A:337:ARG:NH2	2.46	0.49
1:A:319:ALA:HB2	1:A:356:ALA:HB1	1.95	0.49
1:A:389:GLU:HA	1:A:392:TYR:CE2	2.48	0.49
1:B:370:GLU:CG	1:B:371:GLU:H	2.17	0.49
1:A:418:LEU:HD23	1:B:414:LEU:HD12	1.94	0.48
1:A:390:LYS:HG3	1:A:391:ASP:OD1	2.13	0.48
1:A:242:MET:HE3	1:A:294:ALA:CB	2.44	0.48
1:B:388:PRO:HD2	1:B:391:ASP:HB2	1.95	0.48
1:A:354:GLU:OE2	1:A:363:ARG:NH2	2.48	0.47
1:B:411:VAL:O	1:B:414:LEU:HB3	2.14	0.47
1:A:257:GLY:HA2	1:A:260:ARG:HH11	1.79	0.47
1:B:392:TYR:CD2	1:B:392:TYR:C	2.93	0.46
1:B:380:LEU:HD22	1:B:419:LEU:CD1	2.45	0.46
1:A:330:GLY:HA2	1:A:336:GLY:N	2.29	0.46
1:B:383:ARG:HA	1:B:386:ARG:CD	2.45	0.46
1:A:410:VAL:O	1:A:413:ALA:HB3	2.16	0.46
1:B:405:GLU:HB2	1:B:407:ARG:HG2	1.98	0.46
1:A:389:GLU:CD	1:A:390:LYS:N	2.74	0.46
1:A:250:GLU:O	1:A:254:ILE:HG13	2.16	0.45
1:A:392:TYR:HE1	1:A:396:GLN:NE2	2.07	0.45
1:A:246:ARG:HD2	2:A:15:HOH:O	2.16	0.45
1:A:354:GLU:HB2	1:A:360:ARG:HH21	1.82	0.45
1:B:370:GLU:N	1:B:370:GLU:OE2	2.50	0.45
1:B:387:VAL:HA	1:B:388:PRO:HD3	1.80	0.44
1:A:257:GLY:O	1:A:260:ARG:HB2	2.18	0.44
1:A:284:PHE:O	1:A:285:ARG:C	2.61	0.44
1:A:276:GLU:O	1:A:280:VAL:HG23	2.18	0.43
1:A:353:LEU:O	1:A:357:VAL:HB	2.18	0.43
1:A:223:ARG:HB3	1:A:223:ARG:NH1	2.32	0.43
1:A:321:ALA:O	1:A:325:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LYS:HD3	1:A:364:VAL:CG2	2.49	0.43
1:A:354:GLU:CB	1:A:360:ARG:HH21	2.32	0.43
1:A:411:VAL:HG21	1:B:403:PHE:HE2	1.83	0.43
1:B:397:ASP:OD1	1:B:397:ASP:C	2.62	0.43
1:A:403:PHE:CE1	1:B:406:GLY:HA2	2.52	0.42
1:A:226:LEU:HD21	1:A:257:GLY:HA3	2.00	0.42
1:A:237:SER:N	1:A:238:PRO:HD3	2.34	0.42
1:A:221:PRO:CB	1:A:223:ARG:NE	2.77	0.42
1:A:398:PHE:HB3	1:B:377:TRP:CH2	2.54	0.41
1:A:377:TRP:CE2	1:A:381:LEU:HD11	2.55	0.41
1:A:392:TYR:CD1	1:A:392:TYR:C	2.98	0.41
1:A:389:GLU:CD	1:A:390:LYS:H	2.29	0.41
1:B:388:PRO:C	1:B:390:LYS:N	2.75	0.41
1:A:251:THR:HB	1:A:293:VAL:O	2.20	0.41
1:A:280:VAL:HG12	1:A:292:LEU:HD11	2.02	0.41
1:A:242:MET:CE	1:A:294:ALA:HB3	2.48	0.41
1:A:323:GLN:HE22	1:A:357:VAL:HG22	1.86	0.41
1:A:364:VAL:HG12	1:A:365:ASN:O	2.20	0.41
1:A:310:VAL:HG23	1:A:329:THR:HB	2.03	0.40
1:B:383:ARG:HA	1:B:386:ARG:HD2	2.03	0.40
1:A:345:ARG:H	1:A:345:ARG:HG2	1.67	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	202/212 (95%)	195 (96%)	7 (4%)	0	100	100
1	B	48/212 (23%)	43 (90%)	4 (8%)	1 (2%)	5	4
All	All	250/424 (59%)	238 (95%)	11 (4%)	1 (0%)	30	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	407	ARG

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	166/170 (98%)	152 (92%)	14 (8%)	10	14
1	B	40/170 (24%)	35 (88%)	5 (12%)	4	5
All	All	206/340 (61%)	187 (91%)	19 (9%)	8	11

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	GLU
1	A	222	VAL
1	A	223	ARG
1	A	225	ARG
1	A	252	GLU
1	A	286	GLN
1	A	292	LEU
1	A	302	LEU
1	A	323	GLN
1	A	345	ARG
1	A	348	ARG
1	A	357	VAL
1	A	363	ARG
1	A	370	GLU
1	B	384	LEU
1	B	392	TYR
1	B	409	GLU
1	B	417	LEU
1	B	419	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	GLN
1	A	306	GLN

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](#)

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	206/212 (97%)	1.00	25 (12%) 8 9	48, 74, 154, 184	0
1	B	50/212 (23%)	1.76	21 (42%) 0 0	65, 135, 209, 229	0
All	All	256/424 (60%)	1.15	46 (17%) 3 4	48, 80, 182, 229	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	372	VAL	6.2
1	A	404	ALA	4.2
1	A	330	GLY	3.8
1	B	418	LEU	3.8
1	A	394	LEU	3.7
1	A	418	LEU	3.6
1	B	371	GLU	3.4
1	B	377	TRP	3.3
1	A	400	GLY	3.2
1	B	373	LEU	3.2
1	A	395	TYR	3.1
1	A	331	ARG	3.0
1	A	211	VAL	3.0
1	B	415	LEU	3.0
1	A	406	GLY	2.9
1	B	376	LYS	2.8
1	A	212	THR	2.8
1	A	345	ARG	2.8
1	B	417	LEU	2.7
1	B	379	HIS	2.6
1	A	222	VAL	2.6
1	A	399	ALA	2.6
1	B	375	ALA	2.6
1	B	378	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	393	ARG	2.5
1	B	414	LEU	2.4
1	A	398	PHE	2.4
1	B	394	LEU	2.4
1	A	360	ARG	2.4
1	A	402	LEU	2.4
1	B	380	LEU	2.4
1	A	387	VAL	2.3
1	A	286	GLN	2.3
1	B	370	GLU	2.3
1	B	419	LEU	2.3
1	A	302	LEU	2.2
1	B	392	TYR	2.2
1	A	304	ILE	2.2
1	A	221	PRO	2.2
1	A	245	THR	2.2
1	A	408	VAL	2.2
1	B	385	ALA	2.2
1	B	381	LEU	2.1
1	B	390	LYS	2.1
1	A	246	ARG	2.0
1	A	343	GLY	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.