



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:22 PM UTC

PDB ID : 4TK3 / pdb\_00004tk3  
Title : Geph E in complex with a GABA receptor alpha3 derived double mutant peptide in spacegroup P21212  
Authors : Kasaragod, V.B.; Maric, H.M.; Schindelin, H.  
Deposited on : 2014-05-25  
Resolution : 2.70 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](mailto: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>.

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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

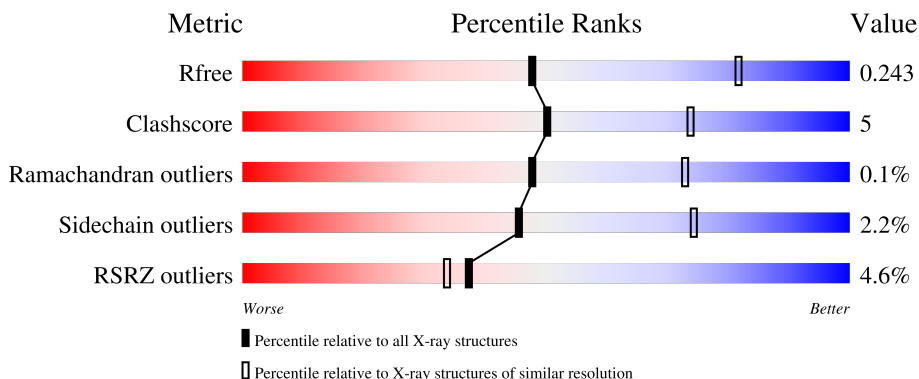
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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  $\geq 3$ , 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	419	 4% 85% 14%
1	B	419	 4% 82% 15%
2	C	11	 18% 36% 36% 9% 18%
2	D	11	 27% 45% 27%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6465 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 Gephyrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	418	3191	2011	553	607	20	0	1	0
1	B	406	3105	1964	536	586	19	0	1	0

- Molecule 2 is a protein called Gamma-aminobutyric acid receptor subunit alpha-3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	9	70	49	9	12	0	0	0
2	D	8	63	44	8	11	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	369	SER	ASN	engineered mutation	UNP P20236
C	374	LEU	THR	engineered mutation	UNP P20236
D	369	SER	ASN	engineered mutation	UNP P20236
D	374	LEU	THR	engineered mutation	UNP P20236

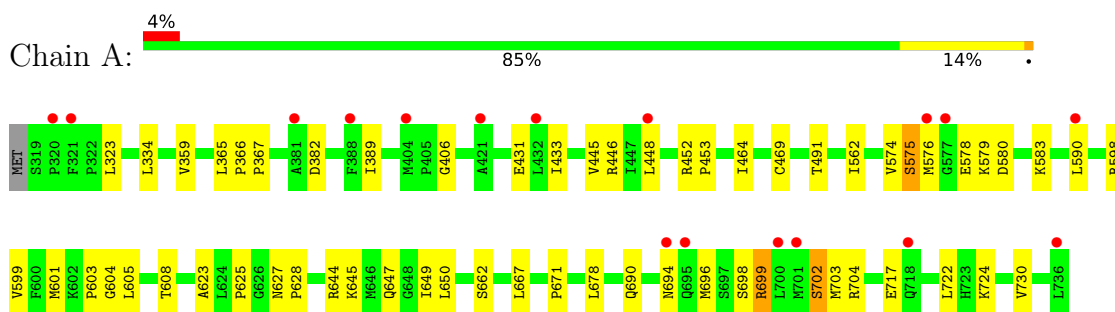
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	18	Total	O	0	0
			18	18		

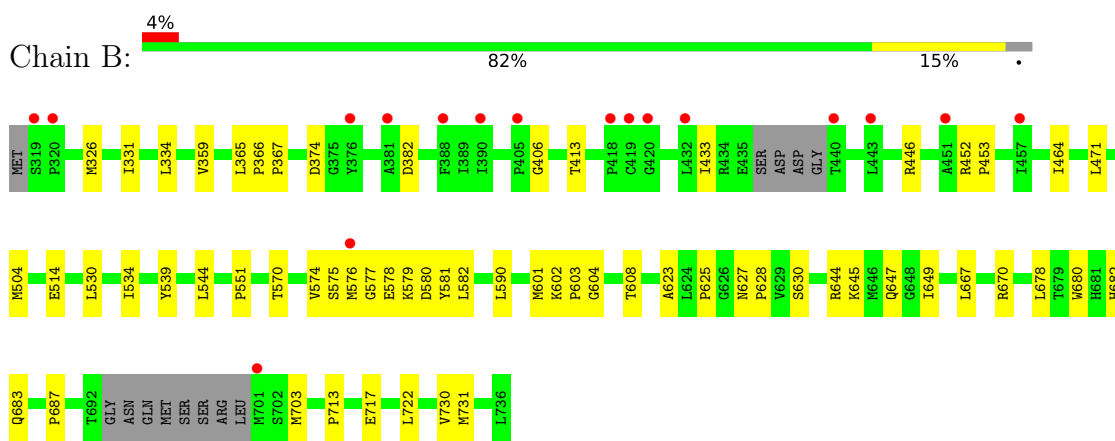
### 3 Residue-property plots [i](#)

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.

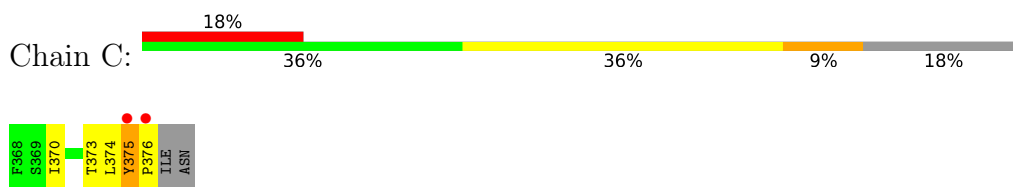
- Molecule 1: Gephyrin



- Molecule 1: Gephyrin



- Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-3



- Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.03Å 157.18Å 51.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.53 – 2.70 48.53 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.53-2.70) 99.9 (48.53-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.229 , 0.267 (Not available) , 0.243	Depositor DCC
$R_{free}$ test set	1277 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.2	Xtrriage
Anisotropy	0.247	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6465	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.31	0/3255	0.72	1/4427 (0.0%)
1	B	0.30	0/3167	0.72	2/4307 (0.0%)
2	C	0.24	0/72	0.48	0/98
2	D	0.22	0/64	0.52	0/86
All	All	0.30	0/6558	0.72	3/8918 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	717	GLU	CB-CA-C	-6.35	109.23	116.54
1	B	577	GLY	N-CA-C	-6.01	98.94	113.18
1	A	575	SER	CB-CA-C	-5.86	109.80	116.54

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	3191	0	3235	33	0
1	B	3105	0	3157	37	0
2	C	70	0	70	3	0
2	D	63	0	63	1	0
3	A	18	0	0	2	0
3	B	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6465	0	6525	68	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 5.

All (68) 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:575:SER:O	1:B:580:ASP:OD2	1.95	0.85
1:A:608:THR:HB	1:A:623:ALA:HB3	1.62	0.82
1:B:608:THR:HB	1:B:623:ALA:HB3	1.67	0.75
1:A:699:ARG:HA	1:A:702:SER:HB2	1.71	0.72
1:A:604:GLY:HA2	1:A:625:PRO:HG2	1.76	0.68
1:A:469:CYS:SG	3:A:807:HOH:O	2.54	0.65
1:B:433:ILE:HD11	1:B:446:ARG:HB2	1.79	0.65
1:A:583:LYS:NZ	1:A:608:THR:OG1	2.27	0.64
1:A:334:LEU:O	1:A:645:LYS:NZ	2.28	0.63
1:B:604:GLY:HA2	1:B:625:PRO:HG2	1.80	0.63
1:B:713:PRO:HG3	2:C:374:LEU:HG	1.83	0.61
1:B:579:LYS:O	1:B:581:TYR:N	2.33	0.59
1:B:334:LEU:O	1:B:645:LYS:NZ	2.28	0.57
1:B:504:MET:HB3	1:B:544:LEU:HB2	1.88	0.56
1:B:574:VAL:HG21	1:B:579:LYS:CB	2.35	0.55
1:A:678:LEU:O	1:A:704:ARG:NH2	2.37	0.55
1:A:562:ILE:HD11	1:A:590:LEU:HD21	1.88	0.55
1:B:574:VAL:HG21	1:B:579:LYS:HB2	1.91	0.52
1:B:667:LEU:HD11	1:B:722:LEU:HD13	1.90	0.52
1:A:575:SER:O	1:A:580:ASP:CG	2.53	0.51
1:A:667:LEU:HD11	1:A:722:LEU:HD13	1.92	0.50
1:A:644:ARG:HB3	1:A:649:ILE:HD12	1.94	0.50
1:A:359:VAL:N	3:A:807:HOH:O	2.46	0.49
1:A:323:LEU:HD23	1:A:598:ARG:HB3	1.94	0.49
1:A:696:MET:HE3	1:B:464:ILE:HG12	1.95	0.49
1:A:671:PRO:HB3	2:D:371:VAL:HG13	1.94	0.48
1:A:574:VAL:CG2	1:A:579:LYS:O	2.61	0.48
1:A:433:ILE:HD11	1:A:446:ARG:HB2	1.94	0.48
1:B:601:MET:O	1:B:670:ARG:NH2	2.34	0.48
1:A:389:ILE:HD11	1:A:445:VAL:HB	1.96	0.47
1:A:662:SER:O	1:A:724:LYS:HE2	2.15	0.47
1:A:491:THR:HG21	1:B:514:GLU:HG3	1.96	0.47
1:A:650:LEU:HD12	1:B:703:MET:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:VAL:HG21	1:B:579:LYS:HB3	1.97	0.47
2:C:375:TYR:HA	2:C:376:PRO:HD2	1.80	0.47
1:B:326:MET:HG3	2:C:370:ILE:HG23	1.98	0.46
1:B:551:PRO:HD3	1:B:581:TYR:CD1	2.51	0.46
1:B:359:VAL:HB	1:B:471:LEU:HB2	1.97	0.45
1:B:452:ARG:HG2	1:B:453:PRO:HD2	1.99	0.45
1:A:678:LEU:HD21	1:A:730:VAL:HG11	1.98	0.45
1:A:452:ARG:HG2	1:A:453:PRO:HD2	1.99	0.45
1:B:682:HIS:CD2	1:B:683:GLN:HG2	2.52	0.44
1:A:698:SER:O	1:A:702:SER:N	2.51	0.43
1:A:574:VAL:HG23	1:A:579:LYS:O	2.18	0.43
1:B:570:THR:HG23	1:B:623:ALA:HA	2.00	0.43
1:B:365:LEU:HA	1:B:366:PRO:HA	1.86	0.43
1:A:431:GLU:HG3	1:A:448:LEU:HD11	2.01	0.43
1:A:662:SER:HB2	1:A:690:GLN:HA	2.02	0.42
1:A:366:PRO:HA	1:A:367:PRO:HD3	1.91	0.42
1:A:599:VAL:O	1:A:605:LEU:HD12	2.19	0.42
1:B:374:ASP:OD1	1:B:413:THR:N	2.49	0.42
1:B:601:MET:HE2	1:B:603:PRO:O	2.20	0.42
1:B:603:PRO:HB2	1:B:630:SER:OG	2.19	0.42
1:B:530:LEU:O	1:B:534:ILE:HG12	2.19	0.41
1:B:575:SER:OG	1:B:576:MET:N	2.53	0.41
1:A:382:ASP:OD2	1:A:406:GLY:N	2.46	0.41
1:B:680:TRP:CE2	1:B:687:PRO:HB3	2.56	0.41
1:B:602:LYS:HA	1:B:603:PRO:HA	1.78	0.41
1:B:678:LEU:HD21	1:B:730:VAL:HG11	2.01	0.41
1:A:601:MET:HE2	1:A:603:PRO:O	2.20	0.41
1:B:627:ASN:HA	1:B:628:PRO:HD3	1.95	0.41
1:B:534:ILE:HG22	1:B:539:TYR:HB2	2.02	0.41
1:A:365:LEU:HB3	1:A:464:ILE:HB	2.03	0.40
1:B:382:ASP:OD2	1:B:406:GLY:N	2.48	0.40
1:B:731:MET:HE3	1:B:731:MET:HB2	1.85	0.40
1:B:366:PRO:HA	1:B:367:PRO:HD3	1.93	0.40
1:B:644:ARG:HB3	1:B:649:ILE:HD12	2.01	0.40
1:A:627:ASN:HA	1:A:628:PRO:HD3	1.89	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	417/419 (100%)	408 (98%)	8 (2%)	1 (0%)	43	68
1	B	401/419 (96%)	397 (99%)	4 (1%)	0	100	100
2	C	7/11 (64%)	6 (86%)	1 (14%)	0	100	100
2	D	6/11 (54%)	5 (83%)	1 (17%)	0	100	100
All	All	831/860 (97%)	816 (98%)	14 (2%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	694	ASN

### 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	356/356 (100%)	349 (98%)	7 (2%)	48	76
1	B	346/356 (97%)	341 (99%)	5 (1%)	59	82
2	C	8/10 (80%)	6 (75%)	2 (25%)	0	2
2	D	7/10 (70%)	5 (71%)	2 (29%)	0	1
All	All	717/732 (98%)	701 (98%)	16 (2%)	45	74

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	576	MET
1	A	578	GLU
1	A	647	GLN
1	A	699	ARG
1	A	702	SER
1	A	703	MET
1	A	717	GLU
1	B	331	ILE
1	B	578	GLU
1	B	582	LEU
1	B	590	LEU
1	B	647	GLN
2	C	373	THR
2	C	375	TYR
2	D	373	THR
2	D	375	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	512	ASN
1	A	682	HIS
1	A	695	GLN
1	B	512	ASN
1	B	537	HIS
1	B	674	HIS
1	B	682	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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	418/419 (99%)	0.34	17 (4%) 41 37	30, 66, 126, 177	1 (0%)
1	B	406/419 (96%)	0.37	17 (4%) 40 37	25, 66, 127, 179	1 (0%)
2	C	9/11 (81%)	1.05	2 (22%) 2 2	63, 69, 149, 157	0
2	D	8/11 (72%)	1.56	3 (37%) 1 0	67, 76, 108, 115	0
All	All	841/860 (97%)	0.37	39 (4%) 37 34	25, 67, 127, 179	2 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	700	LEU	4.5
1	B	418	PRO	3.8
1	B	388	PHE	3.8
1	A	432	LEU	3.8
2	D	374	LEU	3.6
1	A	448	LEU	3.4
1	A	576	MET	3.3
1	A	694	ASN	3.0
2	C	376	PRO	3.0
2	C	375	TYR	3.0
1	A	404	MET	2.9
1	B	451	ALA	2.9
1	A	695	GLN	2.9
1	B	320	PRO	2.8
1	B	319	SER	2.7
1	A	701	MET	2.7
1	B	381	ALA	2.7
1	B	420	GLY	2.6
1	B	576	MET	2.5
1	B	432	LEU	2.5
1	B	419	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	701	MET	2.4
1	A	320	PRO	2.4
1	A	736	LEU	2.4
1	B	405	PRO	2.3
1	A	381	ALA	2.3
1	B	457	ILE	2.3
1	A	388	PHE	2.2
1	B	440	THR	2.2
1	A	718	GLN	2.1
1	B	443	LEU	2.1
1	A	421	ALA	2.1
2	D	372	GLY	2.1
1	A	577	GLY	2.1
1	B	376	TYR	2.1
1	A	590	LEU	2.0
1	B	390	ILE	2.0
1	A	321	PHE	2.0
2	D	375	TYR	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.