Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:33 PM GMT

PDB ID : 4TK3
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)

The following versions of software and data (see references (i)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance (i)

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.
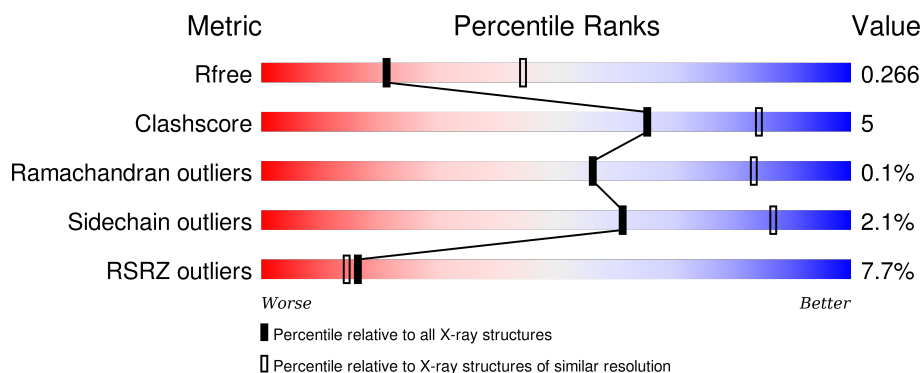
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	6% / 85% / 14%
1	B	419	9% / 83% / 14% / ·
2	C	11	18% / 36% / 36% / 9% / 18%
2	D	11	18% / 45% / 27% / 27%

2 Entry composition (i)

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
1	A	418	Total	C	N	O	S	0	1	0
			3191	2011	553	607	20			
1	B	406	Total	C	N	O	S	0	1	0
			3105	1964	536	586	19			

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

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

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 ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
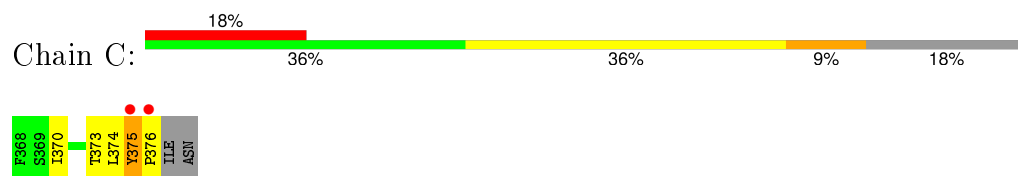
- Molecule 1: Gephyrin
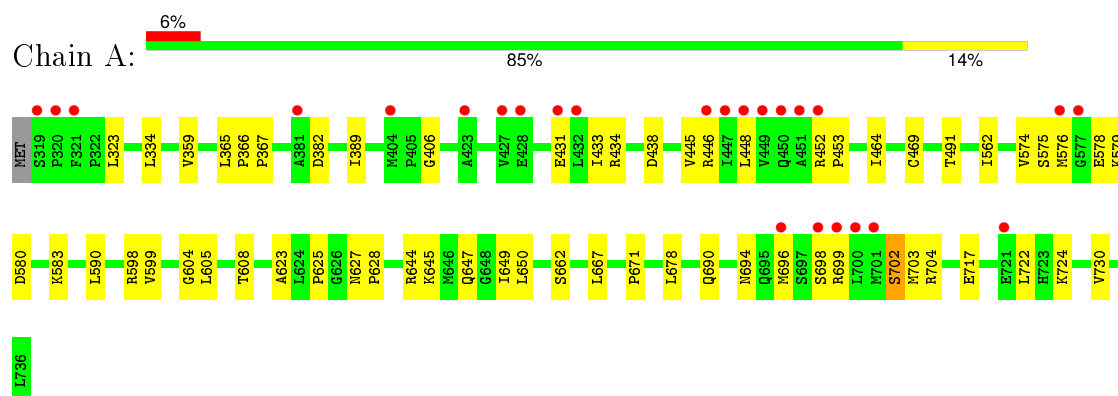
- Molecule 1: Gephyrin
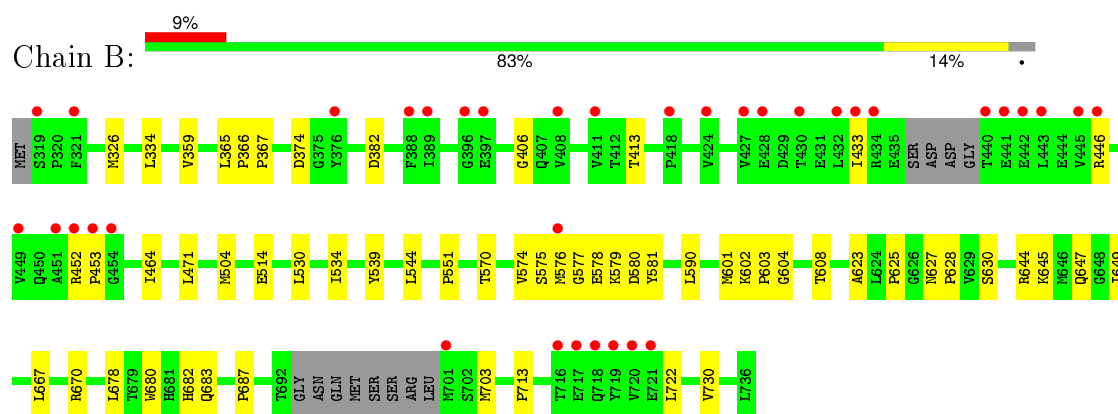
- Molecule 2: Gamma-aminobutyric acid receptor subunit alpha-3

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

F368 V371 G372 T373 L374 Y375 PRO ILE ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	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) 100.0 (48.53-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.229 , 0.267 0.235 , 0.266	Depositor DCC
R_{free} test set	1277 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	56.2	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 25090 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6465	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage'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.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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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	0.24	0/3255	0.39	0/4427
1	B	0.22	0/3167	0.40	1/4307 (0.0%)
2	C	0.23	0/72	0.38	0/98
2	D	0.23	0/64	0.33	0/86
All	All	0.23	0/6558	0.40	1/8918 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	577	GLY	N-CA-C	-5.66	98.94	113.10

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	32	0
1	B	3105	0	3157	35	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
All	All	6465	0	6525	65	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 (65) 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:A:334:LEU:O	1:A:645:LYS:NZ	2.28	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: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:A:696:MET:HE3	1:B:464:ILE:HG12	1.92	0.52
1:B:667:LEU:HD11	1:B:722:LEU:HD13	1.90	0.52
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: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
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:A:575:SER:O	1:A:580:ASP:CG	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:603:PRO:HB2	1:B:630:SER:OG	2.19	0.42
1:B:374:ASP:OD1	1:B:413:THR:N	2.49	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:B:680:TRP:CE2	1:B:687:PRO:HB3	2.56	0.41
1:A:382:ASP:OD2	1:A:406:GLY:N	2.46	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: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: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%)	52	80
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%)	56	83

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%)	348 (98%)	8 (2%)	60	86
1	B	346/356 (97%)	343 (99%)	3 (1%)	84	95
2	C	8/10 (80%)	6 (75%)	2 (25%)	1	2
2	D	7/10 (70%)	5 (71%)	2 (29%)	0	1
All	All	717/732 (98%)	702 (98%)	15 (2%)	61	87

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	434	ARG
1	A	438	ASP
1	A	576	MET
1	A	578	GLU
1	A	647	GLN
1	A	702	SER
1	A	703	MET
1	A	717	GLU
1	B	578	GLU
1	B	590	LEU

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Mol	Chain	Res	Type
1	B	647	GLN
2	C	373	THR
2	C	375	TYR
2	D	373	THR
2	D	375	TYR

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

Mol	Chain	Res	Type
1	A	682	HIS
1	B	401	GLN
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 carbohydrates 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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	418/419 (99%)	0.43	25 (5%) 25	24	33, 67, 126, 177	0
1	B	406/419 (96%)	0.51	36 (8%) 12	9	28, 67, 127, 179	0
2	C	9/11 (81%)	1.25	2 (22%) 1	1	63, 69, 149, 157	0
2	D	8/11 (72%)	1.41	2 (25%) 1	1	67, 76, 108, 115	0
All	All	841/860 (97%)	0.49	65 (7%) 16	14	28, 67, 127, 179	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	433	ILE	9.0
2	C	376	PRO	7.3
1	A	700	LEU	7.1
1	B	440	THR	5.9
1	A	448	LEU	5.3
1	A	381	ALA	5.3
1	B	388	PHE	5.0
1	A	701	MET	5.0
1	B	389	ILE	4.9
1	B	319	SER	4.6
1	B	718	GLN	4.6
1	B	434	ARG	4.3
1	B	432	LEU	4.3
1	A	428	GLU	4.1
2	C	375	TYR	3.9
1	B	453	PRO	3.8
1	A	577	GLY	3.7
1	B	720	VAL	3.5
1	B	428	GLU	3.5
1	A	432	LEU	3.5
1	B	719	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	418	PRO	3.4
1	A	699	ARG	3.3
1	A	404	MET	3.3
1	A	452	ARG	3.3
1	A	451	ALA	3.3
1	A	449	VAL	3.2
1	B	446	ARG	3.1
1	A	427	VAL	3.1
1	B	397	GLU	2.9
1	A	321	PHE	2.9
1	B	451	ALA	2.9
2	D	375	TYR	2.8
1	B	454	GLY	2.8
1	B	717	GLU	2.8
1	A	698	SER	2.7
1	B	576	MET	2.7
1	B	445	VAL	2.7
1	B	396	GLY	2.6
1	B	701	MET	2.6
1	A	696	MET	2.6
2	D	374	LEU	2.6
1	B	376	TYR	2.5
1	B	443	LEU	2.5
1	A	447	ILE	2.5
1	B	411	VAL	2.5
1	B	424	VAL	2.4
1	B	716	THR	2.4
1	B	449	VAL	2.3
1	A	431	GLU	2.3
1	B	408	VAL	2.3
1	B	452	ARG	2.3
1	A	576	MET	2.3
1	B	430	THR	2.3
1	A	423	ALA	2.2
1	A	446	ARG	2.2
1	B	721	GLU	2.2
1	A	450	GLN	2.2
1	A	320	PRO	2.1
1	A	319	SER	2.1
1	B	427	VAL	2.1
1	B	321	PHE	2.1
1	B	441	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	442	GLU	2.0
1	A	721	GLU	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 carbohydrates 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.