



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:06 AM UTC

PDB ID : 2XSS / pdb_00002xss
Title : Crystal structure of GAFb from the human phosphodiesterase 5
Authors : Schlicker, C.; Russwurm, M.; Steegborn, C.
Deposited on : 2010-09-30
Resolution : 2.50 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

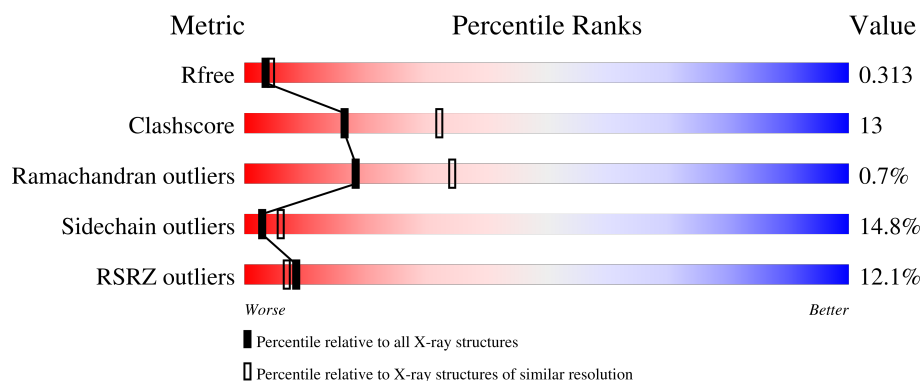
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	181	6% 57% 26% • 14%
1	B	181	15% 54% 24% 5% • 17%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2377 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 CGMP-SPECIFIC 3', 5'-CYCLIC PHOSPHODIESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1215	768	205	230	12			
1	B	150	Total	C	N	O	S	0	0	0
			1162	738	196	216	12			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	MET	-	expression tag	UNP O76074
A	331	ALA	-	expression tag	UNP O76074
A	332	SER	-	expression tag	UNP O76074
A	333	TRP	-	expression tag	UNP O76074
A	334	SER	-	expression tag	UNP O76074
A	335	HIS	-	expression tag	UNP O76074
A	336	PRO	-	expression tag	UNP O76074
A	337	GLN	-	expression tag	UNP O76074
A	338	PHE	-	expression tag	UNP O76074
A	339	GLU	-	expression tag	UNP O76074
A	340	LYS	-	expression tag	UNP O76074
A	341	GLY	-	expression tag	UNP O76074
A	342	ALA	-	expression tag	UNP O76074
A	343	GLU	-	expression tag	UNP O76074
A	344	THR	-	expression tag	UNP O76074
A	345	ALA	-	expression tag	UNP O76074
A	510	ALA	-	expression tag	UNP O76074
B	330	MET	-	expression tag	UNP O76074
B	331	ALA	-	expression tag	UNP O76074
B	332	SER	-	expression tag	UNP O76074
B	333	TRP	-	expression tag	UNP O76074
B	334	SER	-	expression tag	UNP O76074
B	335	HIS	-	expression tag	UNP O76074
B	336	PRO	-	expression tag	UNP O76074
B	337	GLN	-	expression tag	UNP O76074

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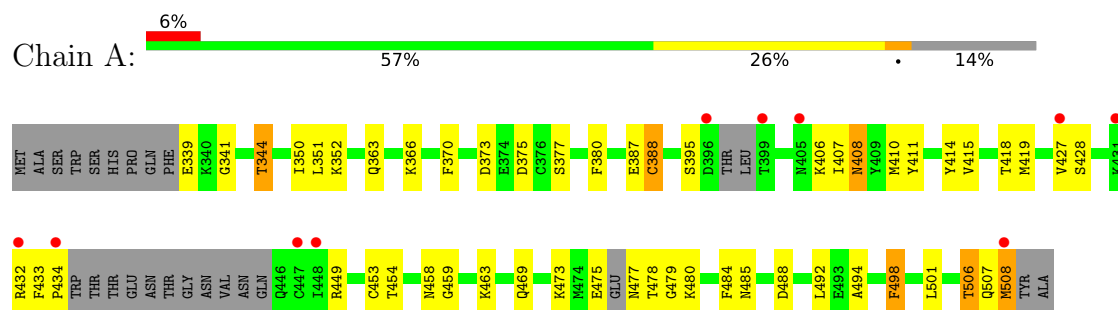
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Chain	Residue	Modelled	Actual	Comment	Reference
B	338	PHE	-	expression tag	UNP O76074
B	339	GLU	-	expression tag	UNP O76074
B	340	LYS	-	expression tag	UNP O76074
B	341	GLY	-	expression tag	UNP O76074
B	342	ALA	-	expression tag	UNP O76074
B	343	GLU	-	expression tag	UNP O76074
B	344	THR	-	expression tag	UNP O76074
B	345	ALA	-	expression tag	UNP O76074
B	510	ALA	-	expression tag	UNP O76074

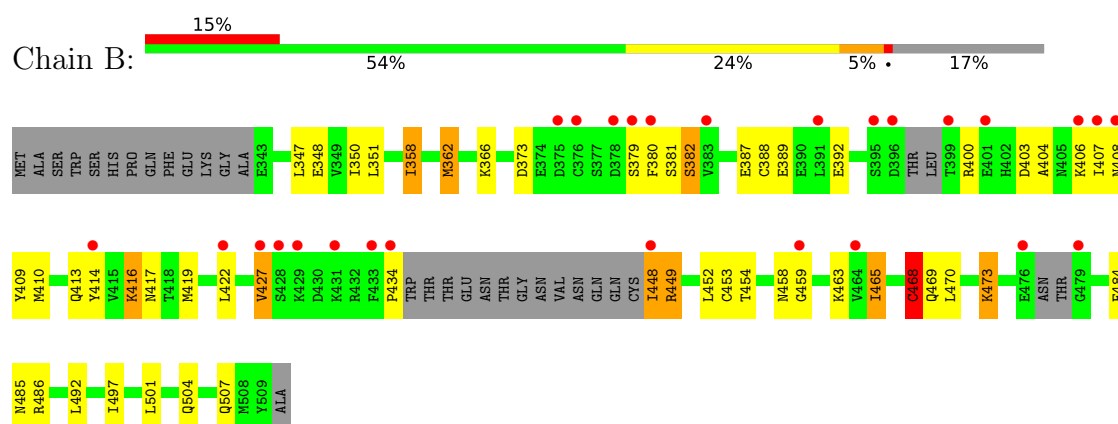
3 Residue-property plots [i](#)

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: CGMP-SPECIFIC 3', 5'-CYCLIC PHOSPHODIESTERASE



• Molecule 1: CGMP-SPECIFIC 3', 5'-CYCLIC PHOSPHODIESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	64.75Å 64.75Å 145.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.39 – 2.50 44.39 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.39-2.50) 99.0 (44.39-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.248 , 0.317 0.244 , 0.313	Depositor DCC
R_{free} test set	633 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2377	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% 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	0.84	0/1230	1.04	1/1647 (0.1%)
1	B	0.90	0/1177	1.05	3/1580 (0.2%)
All	All	0.87	0/2407	1.04	4/3227 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	CYS	CB-CA-C	-7.83	101.72	111.43
1	B	473	LYS	N-CA-C	-5.87	101.72	110.23
1	B	468	CYS	CB-CA-C	-5.40	102.15	110.78
1	B	416	LYS	N-CA-C	-5.03	105.25	111.33

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	1215	0	1204	26	0
1	B	1162	0	1150	36	0
All	All	2377	0	2354	61	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 13.

All (61) 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:410:MET:HE2	1:A:433:PHE:HD1	1.07	1.16
1:A:410:MET:HE2	1:A:433:PHE:CD1	1.98	0.96
1:B:373:ASP:HA	1:B:381:SER:HB3	1.56	0.86
1:B:392:GLU:HB3	1:B:400:ARG:HD3	1.60	0.81
1:B:413:GLN:O	1:B:417:ASN:HB2	1.87	0.73
1:B:413:GLN:O	1:B:417:ASN:CB	2.38	0.72
1:B:410:MET:HE1	1:B:434:PRO:HG2	1.72	0.71
1:B:404:ALA:O	1:B:413:GLN:NE2	2.23	0.71
1:B:388:CYS:O	1:B:389:GLU:HG3	1.93	0.68
1:A:475:GLU:HB3	1:A:479:GLY:HA3	1.79	0.64
1:A:454:THR:OG1	1:A:492:LEU:HD23	1.99	0.62
1:B:448:ILE:C	1:B:449:ARG:HG2	2.26	0.60
1:A:341:GLY:HA2	1:A:344:THR:HG23	1.84	0.58
1:B:413:GLN:O	1:B:417:ASN:CG	2.47	0.57
1:B:387:GLU:HB2	1:B:389:GLU:OE2	2.04	0.56
1:B:458:ASN:HD22	1:B:465:ILE:HD11	1.71	0.55
1:A:373:ASP:OD1	1:A:375:ASP:HB2	2.07	0.55
1:B:473:LYS:HB2	1:B:484:PHE:CE1	2.43	0.53
1:B:366:LYS:HG3	1:B:387:GLU:HB3	1.91	0.53
1:B:452:LEU:HB2	1:B:484:PHE:CG	2.43	0.53
1:B:452:LEU:HD22	1:B:484:PHE:HB3	1.90	0.53
1:B:358:ILE:HD12	1:B:362:MET:HG3	1.90	0.52
1:B:413:GLN:O	1:B:417:ASN:N	2.43	0.51
1:A:373:ASP:OD1	1:A:375:ASP:N	2.43	0.51
1:B:388:CYS:C	1:B:389:GLU:HG3	2.36	0.51
1:B:469:GLN:O	1:B:470:LEU:HD23	2.10	0.51
1:A:410:MET:HE1	1:A:434:PRO:HD2	1.93	0.50
1:A:406:LYS:HB3	1:A:408:ASN:OD1	2.12	0.50
1:A:411:TYR:HB2	1:A:469:GLN:HE21	1.77	0.49
1:B:458:ASN:HB2	1:B:504:GLN:NE2	2.27	0.49
1:B:427:VAL:HB	1:B:449:ARG:O	2.13	0.49
1:B:453:CYS:HA	1:B:468:CYS:O	2.13	0.49
1:A:414:TYR:O	1:A:418:THR:HB	2.13	0.48
1:A:506:THR:C	1:A:508:MET:H	2.21	0.48
1:A:477:ASN:O	1:A:479:GLY:N	2.46	0.48
1:B:392:GLU:CB	1:B:400:ARG:HD3	2.38	0.47
1:B:416:LYS:HE2	1:B:417:ASN:OD1	2.14	0.47
1:B:453:CYS:SG	1:B:469:GLN:HG2	2.55	0.46
1:B:414:TYR:CD1	1:B:422:LEU:HD22	2.51	0.46
1:B:379:SER:OG	1:B:380:PHE:N	2.49	0.46
1:A:494:ALA:HB1	1:B:497:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:PHE:CD1	1:A:498:PHE:C	2.95	0.45
1:B:454:THR:OG1	1:B:492:LEU:HD23	2.17	0.45
1:B:458:ASN:HB2	1:B:504:GLN:HE22	1.82	0.45
1:A:458:ASN:O	1:A:459:GLY:C	2.59	0.45
1:A:418:THR:O	1:A:419:MET:HB2	2.16	0.44
1:B:348:GLU:OE2	1:B:382:SER:OG	2.30	0.44
1:A:415:VAL:HG21	1:A:453:CYS:SG	2.57	0.44
1:A:370:PHE:HB3	1:A:380:PHE:CD1	2.53	0.44
1:A:433:PHE:HA	1:A:434:PRO:HD2	1.74	0.44
1:B:403:ASP:O	1:B:409:TYR:CD2	2.71	0.43
1:B:486:ARG:O	1:B:486:ARG:HD2	2.17	0.43
1:B:458:ASN:HD21	1:B:463:LYS:H	1.67	0.43
1:A:477:ASN:C	1:A:479:GLY:H	2.26	0.42
1:A:411:TYR:HB2	1:A:469:GLN:NE2	2.34	0.42
1:A:366:LYS:HG2	1:A:387:GLU:HB3	2.02	0.41
1:B:501:LEU:HD23	1:B:501:LEU:O	2.20	0.41
1:A:473:LYS:HB2	1:A:484:PHE:CZ	2.55	0.41
1:A:341:GLY:HA2	1:A:344:THR:CG2	2.50	0.41
1:A:485:ASN:O	1:A:488:ASP:HB2	2.21	0.41
1:B:458:ASN:CG	1:B:463:LYS:H	2.29	0.41

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	148/181 (82%)	134 (90%)	13 (9%)	1 (1%)	18	34
1	B	142/181 (78%)	130 (92%)	11 (8%)	1 (1%)	18	34
All	All	290/362 (80%)	264 (91%)	24 (8%)	2 (1%)	18	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	478	THR
1	B	459	GLY

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	135/165 (82%)	113 (84%)	22 (16%)	2	4
1	B	129/165 (78%)	112 (87%)	17 (13%)	4	8
All	All	264/330 (80%)	225 (85%)	39 (15%)	3	6

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	339	GLU
1	A	344	THR
1	A	350	ILE
1	A	351	LEU
1	A	352	LYS
1	A	363	GLN
1	A	377	SER
1	A	388	CYS
1	A	395	SER
1	A	407	ILE
1	A	408	ASN
1	A	427	VAL
1	A	428	SER
1	A	432	ARG
1	A	449	ARG
1	A	463	LYS
1	A	480	LYS
1	A	498	PHE
1	A	501	LEU
1	A	506	THR
1	A	507	GLN
1	A	508	MET

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Mol	Chain	Res	Type
1	B	347	LEU
1	B	350	ILE
1	B	351	LEU
1	B	358	ILE
1	B	362	MET
1	B	382	SER
1	B	406	LYS
1	B	407	ILE
1	B	408	ASN
1	B	419	MET
1	B	427	VAL
1	B	448	ILE
1	B	449	ARG
1	B	465	ILE
1	B	468	CYS
1	B	485	ASN
1	B	507	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	417	ASN
1	A	423	ASN
1	A	469	GLN
1	A	507	GLN
1	B	405	ASN
1	B	408	ASN
1	B	485	ASN
1	B	487	ASN
1	B	490	GLN
1	B	504	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	156/181 (86%)	0.26	10 (6%) 25 22	27, 53, 103, 131	0
1	B	150/181 (82%)	1.00	27 (18%) 3 3	37, 72, 132, 148	0
All	All	306/362 (84%)	0.62	37 (12%) 8 7	27, 63, 125, 148	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	427	VAL	5.0
1	A	447	CYS	4.7
1	B	407	ILE	4.2
1	B	378	ASP	4.0
1	B	434	PRO	4.0
1	B	399	THR	3.9
1	A	399	THR	3.9
1	B	431	LYS	3.8
1	B	396	ASP	3.8
1	A	396	ASP	3.7
1	B	427	VAL	3.5
1	A	448	ILE	3.2
1	B	428	SER	3.1
1	A	405	ASN	3.1
1	B	476	GLU	3.1
1	B	380	PHE	3.1
1	B	479	GLY	3.0
1	B	433	PHE	2.8
1	A	431	LYS	2.7
1	A	434	PRO	2.7
1	A	508	MET	2.6
1	B	375	ASP	2.5
1	B	429	LYS	2.5
1	B	448	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	376	CYS	2.3
1	A	432	ARG	2.3
1	B	414	TYR	2.3
1	B	383	VAL	2.2
1	B	406	LYS	2.2
1	B	395	SER	2.2
1	B	379	SER	2.2
1	B	464	VAL	2.1
1	B	391	LEU	2.1
1	B	459	GLY	2.1
1	B	408	ASN	2.0
1	B	422	LEU	2.0
1	B	401	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 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.