



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:07 PM UTC

PDB ID : 5KCG / pdb_00005kcg
Title : Crystal structure of the aromatic prenyltransferase AtaPT (apo state) from *Aspergillus terreus* A8-4
Authors : Sun, F.; Gao, B.
Deposited on : 2016-06-06
Resolution : 1.90 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

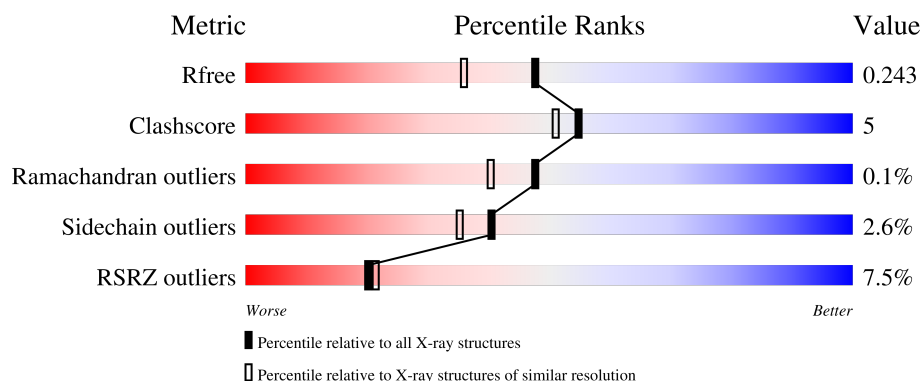
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	419	
1	B	419	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6553 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 aromatic prenyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	0	0
			3156	2041	526	576	13			
1	B	397	Total	C	N	O	S	0	0	0
			3145	2035	522	575	13			

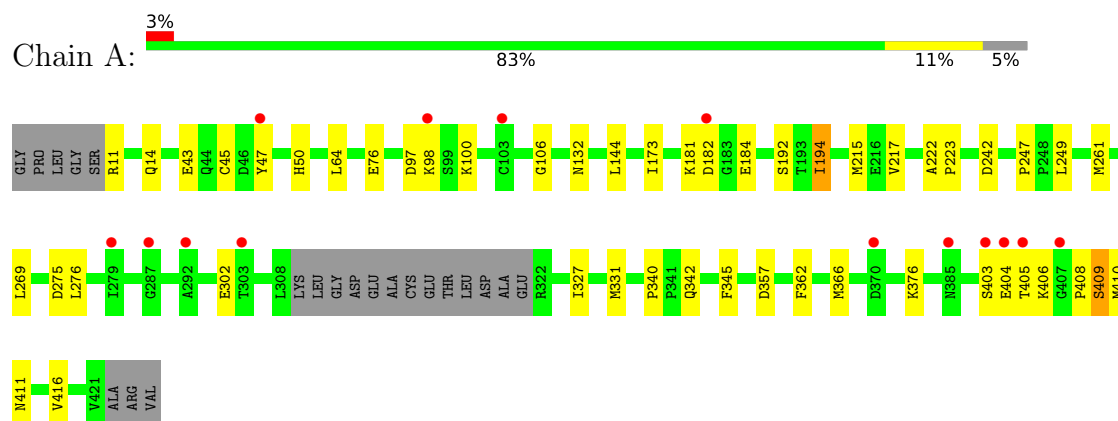
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	148	Total	O	0	0
			148	148		
2	B	104	Total	O	0	0
			104	104		

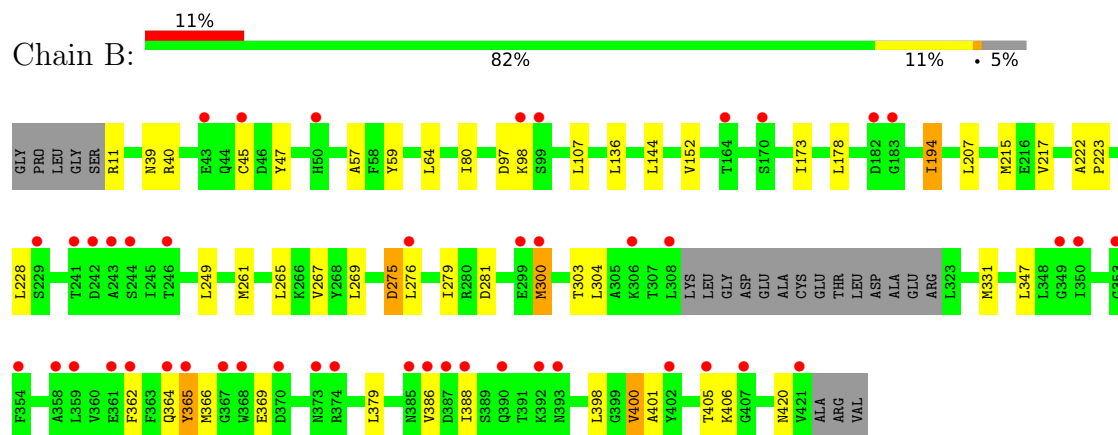
3 Residue-property plots

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: aromatic prenyltransferase



- Molecule 1: aromatic prenyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.20Å 135.81Å 69.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.58 – 1.90 48.58 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.58-1.90) 98.8 (48.58-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.192 , 0.236 0.201 , 0.243	Depositor DCC
R_{free} test set	3491 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6553	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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	7/3236 (0.2%)	1.09	7/4402 (0.2%)
1	B	1.29	11/3225 (0.3%)	1.11	7/4388 (0.2%)
All	All	1.30	18/6461 (0.3%)	1.10	14/8790 (0.2%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	265	LEU	N-CA	-6.15	1.38	1.46
1	A	409	SER	CA-C	-5.86	1.45	1.52
1	B	136	LEU	CA-C	5.74	1.60	1.52
1	A	76	GLU	C-O	-5.59	1.18	1.24
1	B	80	ILE	N-CA	5.58	1.53	1.46
1	B	401	ALA	CA-C	-5.56	1.45	1.52
1	B	267	VAL	N-CA	-5.54	1.39	1.46
1	A	416	VAL	C-O	-5.52	1.17	1.24
1	B	59	TYR	N-CA	-5.47	1.39	1.46
1	B	64	LEU	C-O	-5.37	1.19	1.24
1	B	107	LEU	C-O	-5.32	1.17	1.23
1	A	106	GLY	C-O	-5.23	1.16	1.23
1	B	281	ASP	CA-C	5.21	1.59	1.52
1	B	57	ALA	CA-CB	-5.10	1.45	1.53
1	A	340	PRO	C-O	-5.07	1.20	1.25
1	B	178	LEU	N-CA	-5.04	1.40	1.46
1	A	132	ASN	CG-ND2	-5.03	1.22	1.33
1	A	64	LEU	CA-C	5.03	1.58	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	PRO	CB-CA-C	-5.85	103.78	110.92
1	B	152	VAL	N-CA-C	5.84	118.51	112.90
1	B	300	MET	CB-CA-C	-5.83	101.65	110.92
1	A	345	PHE	CA-C-N	5.64	126.51	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	PHE	C-N-CA	5.64	126.51	120.13
1	B	420	ASN	N-CA-C	-5.52	107.19	114.31
1	A	194	ILE	CA-C-O	5.44	122.33	118.69
1	B	194	ILE	CA-C-N	-5.33	113.14	119.05
1	B	194	ILE	C-N-CA	-5.33	113.14	119.05
1	A	405	THR	N-CA-C	5.23	117.78	111.40
1	B	300	MET	CA-CB-CG	5.19	124.49	114.10
1	A	406	LYS	N-CA-C	5.17	119.44	113.18
1	A	275	ASP	N-CA-C	-5.14	101.44	108.38
1	B	275	ASP	N-CA-C	-5.12	101.47	108.38

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	3156	0	3168	27	0
1	B	3145	0	3155	33	0
2	A	148	0	0	2	0
2	B	104	0	0	2	0
All	All	6553	0	6323	60	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 (60) 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:362:PHE:CZ	1:B:366:MET:HE3	1.81	1.14
1:B:300:MET:HG2	1:B:366:MET:HE1	1.53	0.88
1:A:11:ARG:NH1	1:A:43:GLU:OE2	2.21	0.73
1:B:365:TYR:CE1	1:B:366:MET:HE2	2.25	0.70
1:B:144:LEU:HD22	1:B:215:MET:HE3	1.73	0.69
1:A:144:LEU:HD22	1:A:215:MET:HE3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LEU:CD2	1:B:215:MET:HE3	2.26	0.65
1:B:365:TYR:CD1	1:B:366:MET:HE2	2.31	0.65
1:A:50:HIS:HB2	2:A:514:HOH:O	1.98	0.62
1:A:144:LEU:CD2	1:A:215:MET:HE3	2.30	0.62
1:A:357:ASP:OD1	1:A:376:LYS:NZ	2.27	0.60
1:B:304:LEU:HD23	1:B:400:VAL:HG21	1.84	0.59
1:B:362:PHE:CE1	1:B:366:MET:HE3	2.34	0.59
1:B:365:TYR:CD1	1:B:365:TYR:C	2.79	0.59
1:A:342:GLN:HE22	1:A:411:ASN:HD22	1.48	0.59
1:B:11:ARG:CD	2:B:514:HOH:O	2.51	0.57
1:A:11:ARG:HB2	1:A:14:GLN:OE1	2.04	0.57
1:A:217:VAL:HG23	1:A:261:MET:CE	2.35	0.57
1:A:276:LEU:CD2	1:A:302:GLU:HG2	2.36	0.56
1:B:304:LEU:CD2	1:B:400:VAL:HG21	2.35	0.56
1:B:11:ARG:HD3	2:B:514:HOH:O	2.06	0.56
1:B:228:LEU:CD2	1:B:331:MET:CE	2.84	0.56
1:B:228:LEU:HD23	1:B:331:MET:HE1	1.87	0.56
1:A:11:ARG:NH1	1:A:43:GLU:CD	2.65	0.55
1:B:228:LEU:CD2	1:B:331:MET:HE1	2.38	0.53
1:B:217:VAL:HG12	1:B:261:MET:HE2	1.90	0.53
1:B:300:MET:CG	1:B:366:MET:HE1	2.33	0.53
1:A:331:MET:HB2	2:A:532:HOH:O	2.09	0.52
1:B:303:THR:HG21	1:B:365:TYR:CD2	2.45	0.52
1:A:276:LEU:HD22	1:A:302:GLU:HG2	1.93	0.50
1:A:11:ARG:HH12	1:A:43:GLU:CD	2.19	0.50
1:A:362:PHE:CD2	1:A:410:MET:HE1	2.48	0.48
1:A:342:GLN:HE22	1:A:411:ASN:ND2	2.12	0.48
1:A:45:CYS:HB2	1:A:47:TYR:CE1	2.49	0.47
1:A:404:GLU:N	1:A:404:GLU:CD	2.73	0.47
1:A:45:CYS:HB2	1:A:47:TYR:CD1	2.49	0.47
1:A:342:GLN:NE2	1:A:411:ASN:HD22	2.13	0.47
1:B:379:LEU:HD23	1:B:388:ILE:HD12	1.97	0.46
1:B:45:CYS:HB2	1:B:47:TYR:CE1	2.51	0.45
1:B:45:CYS:HB2	1:B:47:TYR:CD1	2.51	0.45
1:A:222:ALA:HB3	1:A:223:PRO:HD3	1.98	0.45
1:B:39:ASN:C	1:B:39:ASN:HD22	2.24	0.45
1:A:249:LEU:O	1:A:269:LEU:HA	2.17	0.44
1:B:347:LEU:HD11	1:B:398:LEU:HB2	1.99	0.44
1:B:207:LEU:C	1:B:207:LEU:HD12	2.43	0.44
1:A:242:ASP:OD1	1:A:242:ASP:C	2.60	0.43
1:A:404:GLU:N	1:A:404:GLU:OE1	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:GLN:HG2	1:B:369:GLU:OE1	2.19	0.43
1:B:228:LEU:HD23	1:B:331:MET:CE	2.47	0.43
1:B:40:ARG:HA	1:B:40:ARG:HD3	1.86	0.43
1:A:217:VAL:HG23	1:A:261:MET:HE2	2.01	0.42
1:B:222:ALA:HB3	1:B:223:PRO:HD3	2.00	0.42
1:B:249:LEU:O	1:B:269:LEU:HA	2.19	0.42
1:B:275:ASP:OD1	1:B:275:ASP:C	2.63	0.42
1:A:404:GLU:CD	1:A:404:GLU:H	2.25	0.41
1:A:366:MET:HE1	1:A:408:PRO:HB2	2.03	0.41
1:B:144:LEU:CD2	1:B:215:MET:CE	2.98	0.41
1:B:405:THR:HB	1:B:406:LYS:HG3	2.03	0.41
1:A:97:ASP:OD1	1:A:97:ASP:C	2.64	0.41
1:B:97:ASP:OD1	1:B:97:ASP:C	2.65	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	394/419 (94%)	389 (99%)	4 (1%)	1 (0%)	36	29
1	B	393/419 (94%)	387 (98%)	6 (2%)	0	100	100
All	All	787/838 (94%)	776 (99%)	10 (1%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	ASP

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	343/358 (96%)	333 (97%)	10 (3%)	37	31
1	B	342/358 (96%)	334 (98%)	8 (2%)	44	40
All	All	685/716 (96%)	667 (97%)	18 (3%)	40	35

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	LYS
1	A	100	LYS
1	A	173	ILE
1	A	181	LYS
1	A	184	GLU
1	A	192	SER
1	A	194	ILE
1	A	327	ILE
1	A	403	SER
1	A	409	SER
1	B	98	LYS
1	B	173	ILE
1	B	194	ILE
1	B	276	LEU
1	B	279	ILE
1	B	365	TYR
1	B	386	VAL
1	B	400	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	44	GLN
1	A	85	HIS
1	A	88	HIS

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Mol	Chain	Res	Type
1	A	342	GLN
1	B	27	GLN
1	B	60	HIS
1	B	85	HIS
1	B	149	ASN
1	B	151	GLN
1	B	172	ASN
1	B	364	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	398/419 (94%)	0.26	14 (3%) 47 50	13, 25, 45, 82	0
1	B	397/419 (94%)	0.73	46 (11%) 9 10	16, 31, 52, 78	0
All	All	795/838 (94%)	0.49	60 (7%) 20 21	13, 28, 50, 82	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	421	VAL	5.1
1	B	308	LEU	3.9
1	B	99	SER	3.8
1	B	354	PHE	3.7
1	B	365	TYR	3.4
1	B	182	ASP	3.4
1	B	370	ASP	3.3
1	A	98	LYS	3.2
1	B	393	ASN	3.2
1	A	403	SER	3.2
1	A	405	THR	3.1
1	B	244	SER	3.1
1	B	405	THR	3.0
1	B	229	SER	2.9
1	B	390	GLN	2.9
1	B	246	THR	2.8
1	B	392	LYS	2.8
1	B	358	ALA	2.8
1	B	368	TRP	2.8
1	B	243	ALA	2.7
1	A	287	GLY	2.6
1	A	103	CYS	2.6
1	B	364	GLN	2.6
1	B	45	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	407	GLY	2.6
1	B	350	ILE	2.5
1	B	353	GLY	2.5
1	A	404	GLU	2.5
1	B	43	GLU	2.4
1	B	299	GLU	2.4
1	B	386	VAL	2.4
1	B	374	ARG	2.4
1	A	182	ASP	2.3
1	B	387	ASP	2.3
1	B	276	LEU	2.3
1	B	388	ILE	2.3
1	B	300	MET	2.3
1	B	359	LEU	2.3
1	B	98	LYS	2.3
1	B	361	GLU	2.2
1	A	279	ILE	2.2
1	B	385	ASN	2.2
1	B	306	LYS	2.2
1	B	373	ASN	2.2
1	B	241	THR	2.2
1	B	50	HIS	2.2
1	B	402	TYR	2.1
1	B	349	GLY	2.1
1	B	367	GLY	2.1
1	B	362	PHE	2.0
1	A	303	THR	2.0
1	A	292	ALA	2.0
1	A	370	ASP	2.0
1	B	242	ASP	2.0
1	B	170	SER	2.0
1	B	164	THR	2.0
1	B	183	GLY	2.0
1	A	47	TYR	2.0
1	A	385	ASN	2.0
1	B	407	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.