



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:56 PM UTC

PDB ID : 5I5I / pdb_00005i5i
Title : Shewanella denitrificans nitrous oxide reductase, app form
Authors : Schneider, L.K.; Einsle, O.
Deposited on : 2016-02-15
Resolution : 2.14 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

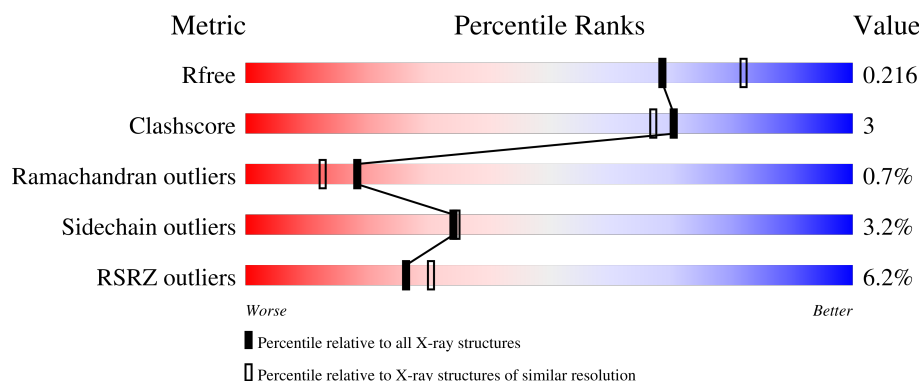
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	636	5% 75% 9% 15%
1	B	636	5% 76% 8% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8589 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 Nitrous-oxide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4254	2687	742	795	30			
1	B	537	Total	C	N	O	S	0	2	0
			4243	2682	741	790	30			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	629	LEU	-	expression tag	UNP Q12M27
A	630	GLU	-	expression tag	UNP Q12M27
A	631	HIS	-	expression tag	UNP Q12M27
A	632	HIS	-	expression tag	UNP Q12M27
A	633	HIS	-	expression tag	UNP Q12M27
A	634	HIS	-	expression tag	UNP Q12M27
A	635	HIS	-	expression tag	UNP Q12M27
A	636	HIS	-	expression tag	UNP Q12M27
B	629	LEU	-	expression tag	UNP Q12M27
B	630	GLU	-	expression tag	UNP Q12M27
B	631	HIS	-	expression tag	UNP Q12M27
B	632	HIS	-	expression tag	UNP Q12M27
B	633	HIS	-	expression tag	UNP Q12M27
B	634	HIS	-	expression tag	UNP Q12M27
B	635	HIS	-	expression tag	UNP Q12M27
B	636	HIS	-	expression tag	UNP Q12M27

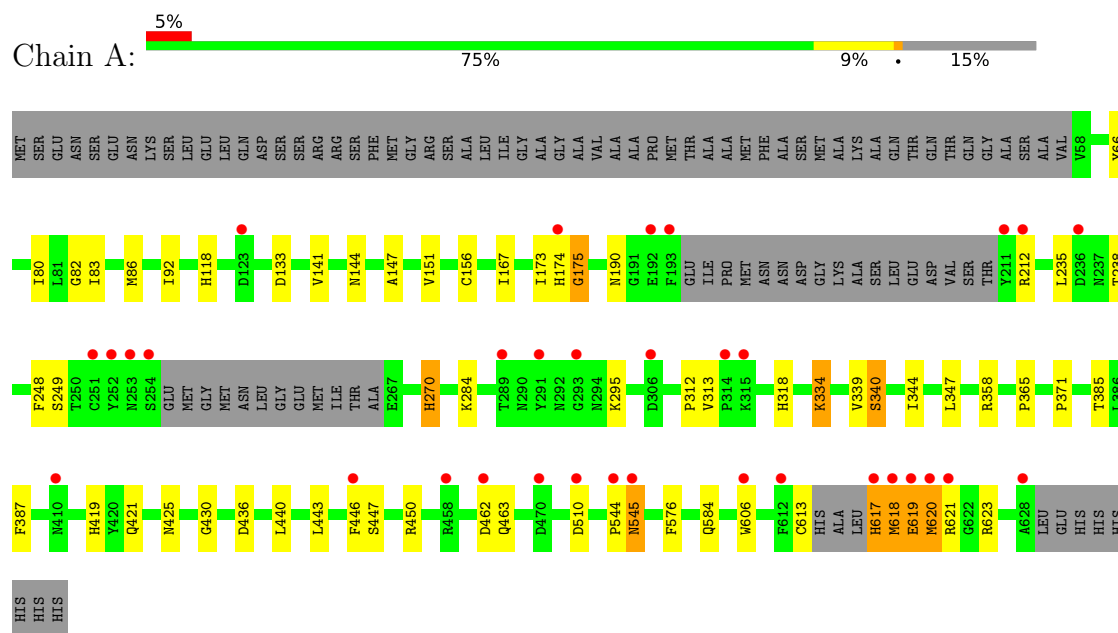
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	50	Total	O	0	0
			50	50		
2	B	42	Total	O	0	0
			42	42		

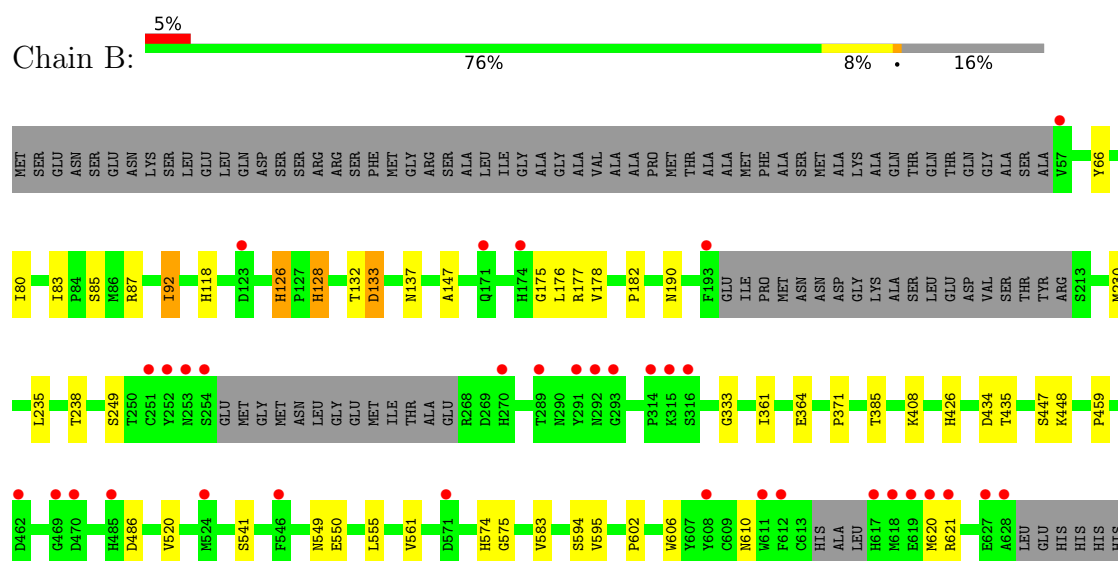
3 Residue-property plots

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: Nitrous-oxide reductase



• Molecule 1: Nitrous-oxide reductase



HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.08Å 121.62Å 178.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.54 – 2.14 100.54 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.3 (100.54-2.14) 100.0 (100.54-2.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.237 , 0.286 (Not available) , 0.216	Depositor DCC
R_{free} test set	8559 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	2.4	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8589	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8313e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	1.04	0/4352	1.03	4/5889 (0.1%)
1	B	1.03	3/4348 (0.1%)	1.03	10/5885 (0.2%)
All	All	1.03	3/8700 (0.0%)	1.03	14/11774 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	ILE	N-CA	-5.96	1.41	1.46
1	B	520	VAL	C-O	-5.32	1.18	1.24
1	B	361	ILE	C-O	-5.29	1.18	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	545	ASN	N-CA-C	6.22	118.52	109.07
1	A	147	ALA	N-CA-C	6.10	118.73	111.71
1	B	364	GLU	CA-C-N	-5.95	113.02	120.51
1	B	364	GLU	C-N-CA	-5.95	113.02	120.51
1	B	333	GLY	N-CA-C	5.55	120.52	113.24
1	B	118	HIS	N-CA-C	5.51	119.11	112.38
1	A	118	HIS	N-CA-C	5.45	117.97	111.71
1	B	132	THR	CA-C-N	5.42	131.45	121.70
1	B	132	THR	C-N-CA	5.42	131.45	121.70
1	B	126	HIS	CB-CA-C	-5.30	104.92	110.33
1	A	430	GLY	N-CA-C	5.23	119.01	112.73
1	B	235	LEU	N-CA-C	5.06	117.77	110.28
1	B	132	THR	CB-CA-C	-5.03	102.89	110.24
1	B	147	ALA	N-CA-C	5.03	117.50	111.71

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	4254	0	4154	32	0
1	B	4243	0	4149	25	0
2	A	50	0	0	1	0
2	B	42	0	0	1	0
All	All	8589	0	8303	57	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 3.

All (57) 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:80:ILE:HD11	1:B:92:ILE:HD11	1.69	0.74
1:A:80:ILE:HD11	1:A:92:ILE:HD11	1.78	0.65
1:A:238:THR:HG22	1:A:249:SER:OG	1.96	0.64
1:B:190:ASN:OD1	1:B:238:THR:HG23	1.97	0.64
1:A:270:HIS:ND1	2:A:701:HOH:O	2.31	0.61
1:A:419:HIS:H	1:A:463:GLN:HE22	1.47	0.60
1:B:447:SER:OG	1:B:459:PRO:O	2.18	0.58
1:B:238:THR:HG22	1:B:249:SER:OG	2.02	0.58
1:B:128:HIS:CD2	1:B:178:VAL:HG22	2.42	0.54
1:A:190:ASN:HD21	1:A:238:THR:HG23	1.72	0.54
1:A:151:VAL:HG23	1:A:167:ILE:HD11	1.91	0.53
1:B:434:ASP:O	1:B:435:THR:C	2.51	0.53
1:A:190:ASN:ND2	1:A:238:THR:HG23	2.24	0.52
1:B:549:ASN:ND2	2:B:701:HOH:O	2.36	0.52
1:A:387:PHE:O	1:A:421:GLN:NE2	2.42	0.52
1:A:235:LEU:HD22	1:A:249:SER:HB2	1.93	0.51
1:A:545:ASN:HA	1:A:620:MET:HG2	1.92	0.51
1:B:133:ASP:HB3	1:B:182:PRO:O	2.11	0.50
1:B:128:HIS:HD2	1:B:178:VAL:HG22	1.76	0.50
1:B:606:TRP:CE3	1:B:621:ARG:HD3	2.47	0.49
1:A:66:TYR:OH	1:A:436:ASP:OD2	2.25	0.49
1:A:167:ILE:HD12	1:A:167:ILE:N	2.27	0.49
1:B:583:VAL:HG13	1:B:595:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:TYR:HB2	1:B:83:ILE:HB	1.95	0.49
1:B:176:LEU:HD23	1:B:176:LEU:C	2.39	0.47
1:A:425:ASN:HB2	1:A:440:LEU:HD11	1.96	0.47
1:A:174:HIS:O	1:A:175:GLY:O	2.32	0.47
1:A:312:PRO:HG2	1:A:358:ARG:HD3	1.98	0.46
1:A:313:VAL:HG23	1:A:340:SER:OG	2.16	0.46
1:B:408:LYS:HA	1:B:408:LYS:HE2	1.98	0.46
1:A:82:GLY:O	1:A:86:MET:N	2.48	0.45
1:A:421:GLN:HG2	1:A:446:PHE:HD2	1.82	0.45
1:B:85:SER:HB3	1:B:87:ARG:HG3	1.99	0.45
1:B:177:ARG:HG3	1:B:238:THR:O	2.17	0.45
1:A:617:HIS:CG	1:A:618:MET:N	2.85	0.45
1:B:426[A]:HIS:CE1	1:B:486:ASP:OD1	2.70	0.45
1:B:426[A]:HIS:NE2	1:B:486:ASP:OD1	2.51	0.44
1:B:555:LEU:HD13	1:B:602:PRO:HG3	1.99	0.44
1:A:447:SER:O	1:A:450:ARG:HG2	2.18	0.43
1:B:575:GLY:HA3	1:B:610:ASN:OD1	2.18	0.43
1:A:66:TYR:HB2	1:A:83:ILE:HB	2.01	0.43
1:A:371:PRO:HA	1:A:385:THR:O	2.18	0.43
1:B:541:SER:OG	1:B:574:HIS:ND1	2.44	0.42
1:A:619:GLU:O	1:A:621:ARG:N	2.52	0.42
1:A:270:HIS:HA	1:A:313:VAL:HG12	2.01	0.42
1:B:126:HIS:CD2	1:B:175:GLY:HA2	2.54	0.42
1:B:137:ASN:OD1	1:B:137:ASN:C	2.62	0.42
1:A:318:HIS:HB2	1:A:334:LYS:HD3	2.02	0.42
1:A:606:TRP:CH2	1:A:623:ARG:HD3	2.55	0.42
1:A:141:VAL:HG23	1:A:156:CYS:SG	2.60	0.42
1:B:561:VAL:O	1:B:594:SER:HA	2.20	0.41
1:A:339:VAL:O	1:A:365:PRO:HD2	2.21	0.41
1:A:443:LEU:HD22	1:A:462:ASP:OD1	2.20	0.41
1:A:144:ASN:HD22	1:A:173:ILE:HG22	1.86	0.41
1:A:576:PHE:O	1:A:584:GLN:HA	2.21	0.40
1:A:344:ILE:HG23	1:A:347:LEU:HD12	2.03	0.40
1:B:371:PRO:HA	1:B:385:THR:O	2.22	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	531/636 (84%)	505 (95%)	21 (4%)	5 (1%)	14	8
1	B	531/636 (84%)	502 (94%)	27 (5%)	2 (0%)	30	26
All	All	1062/1272 (84%)	1007 (95%)	48 (4%)	7 (1%)	18	13

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	620	MET
1	A	175	GLY
1	A	618	MET
1	A	620	MET
1	A	133	ASP
1	A	334	LYS
1	B	448	LYS

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	331/541 (61%)	320 (97%)	11 (3%)	33	33
1	B	135/541 (25%)	131 (97%)	4 (3%)	36	37
All	All	466/1082 (43%)	451 (97%)	15 (3%)	34	35

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

Mol	Chain	Res	Type
1	A	212	ARG
1	A	248	PHE
1	A	270	HIS
1	A	284	LYS
1	A	295	LYS
1	A	340	SER
1	A	510	ASP
1	A	544	PRO
1	A	613	CYS
1	A	617	HIS
1	A	619	GLU
1	B	128	HIS
1	B	133	ASP
1	B	230	MET
1	B	550	GLU

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	290	ASN
1	A	321	ASN
1	A	410	ASN
1	A	421	GLN
1	A	461	ASN
1	A	463	GLN
1	A	498	GLN
1	A	584	GLN
1	A	617	HIS
1	B	128	HIS
1	B	171	GLN
1	B	270	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	539/636 (84%)	0.56	33 (6%) 27 31	18, 32, 59, 93	0
1	B	537/636 (84%)	0.61	34 (6%) 26 30	13, 33, 60, 87	2 (0%)
All	All	1076/1272 (84%)	0.59	67 (6%) 26 30	13, 32, 60, 93	2 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	612	PHE	5.4
1	A	251	CYS	4.8
1	A	618	MET	4.7
1	B	618	MET	4.3
1	A	211	TYR	4.2
1	A	617	HIS	4.2
1	B	293	GLY	4.1
1	A	236	ASP	4.1
1	B	620	MET	3.7
1	A	252	TYR	3.6
1	B	254	SER	3.5
1	B	251	CYS	3.5
1	B	252	TYR	3.5
1	B	193	PHE	3.4
1	A	612	PHE	3.4
1	A	254	SER	3.3
1	B	292	ASN	3.2
1	A	628	ALA	3.1
1	A	620	MET	3.1
1	B	291	TYR	3.1
1	B	546	PHE	3.1
1	B	619	GLU	3.1
1	A	212	ARG	2.9
1	A	545	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	291	TYR	2.8
1	B	57	VAL	2.8
1	A	123	ASP	2.7
1	A	462	ASP	2.7
1	B	628	ALA	2.7
1	A	510	ASP	2.7
1	B	617	HIS	2.6
1	B	316	SER	2.6
1	B	462	ASP	2.6
1	B	174[A]	HIS	2.6
1	A	315	LYS	2.5
1	A	192	GLU	2.5
1	B	314	PRO	2.5
1	A	619	GLU	2.4
1	A	314	PRO	2.4
1	B	123	ASP	2.4
1	B	315	LYS	2.4
1	A	621	ARG	2.3
1	A	193	PHE	2.3
1	A	458	ARG	2.3
1	B	469	GLY	2.3
1	A	289	THR	2.2
1	B	571	ASP	2.2
1	B	627	GLU	2.2
1	B	524	MET	2.2
1	B	608	TYR	2.2
1	A	253	ASN	2.2
1	B	621	ARG	2.2
1	A	306	ASP	2.2
1	B	289	THR	2.2
1	A	293	GLY	2.1
1	B	270	HIS	2.1
1	A	470	ASP	2.1
1	A	606	TRP	2.1
1	B	611	TRP	2.1
1	A	544	PRO	2.1
1	A	446	PHE	2.1
1	A	410	ASN	2.0
1	B	253	ASN	2.0
1	B	470	ASP	2.0
1	B	171	GLN	2.0
1	A	174	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	485	HIS	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.