



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2016 – 02:23 AM EDT

PDB ID : 5I5I
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

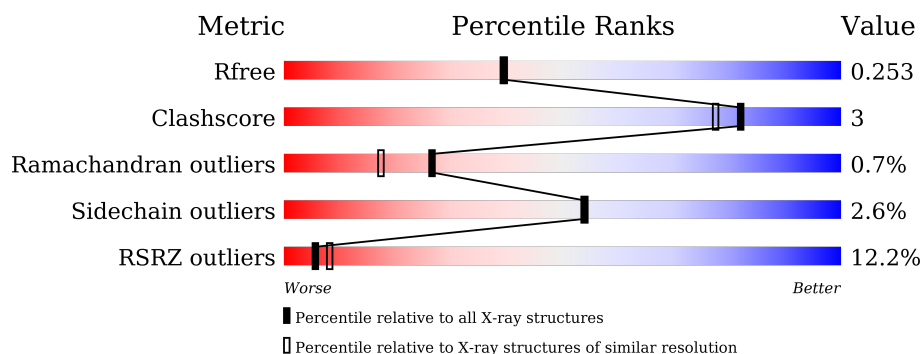
1 Overall quality at a glance

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}	91344	1693 (2.16-2.12)
Clashscore	102246	1824 (2.16-2.12)
Ramachandran outliers	100387	1798 (2.16-2.12)
Sidechain outliers	100360	1798 (2.16-2.12)
RSRZ outliers	91569	1699 (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 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 $\leq 5\%$. 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	<div> <div>11%</div> <div> <div></div> <div>74%</div> <div>9%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	636	<div> <div>10%</div> <div> <div></div> <div>77%</div> <div>7%</div> <div>16%</div> </div> </div>

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

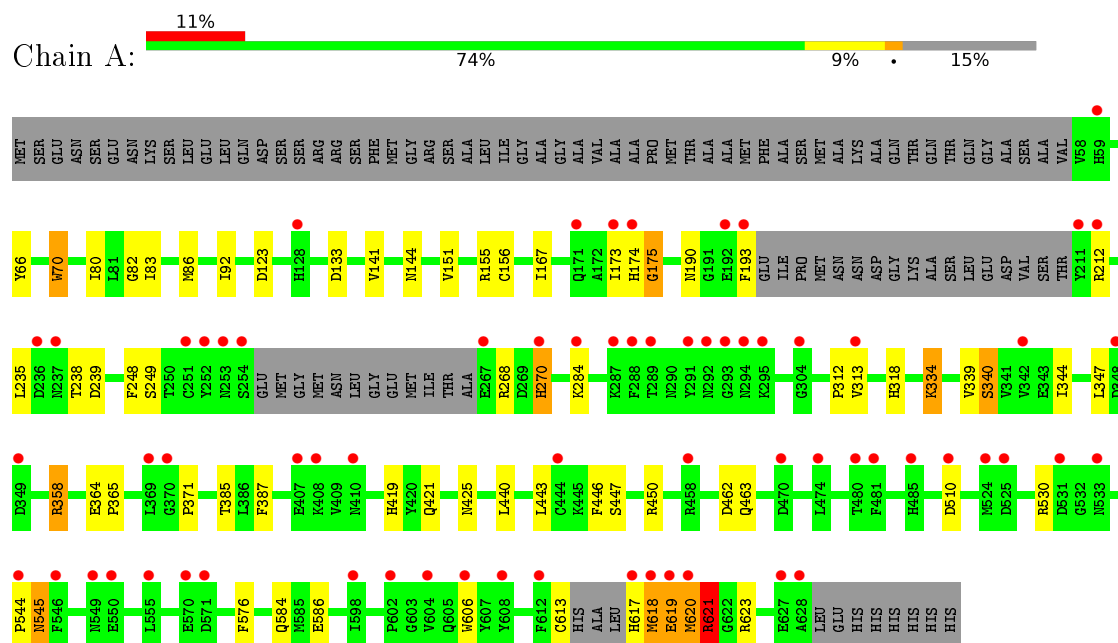
- Molecule 2 is water.

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

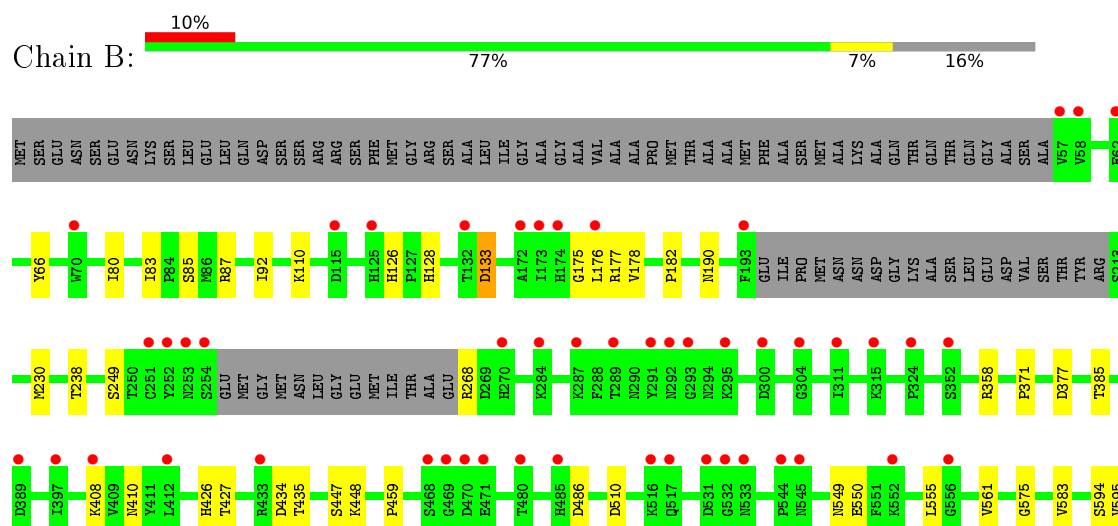
3 Residue-property plots

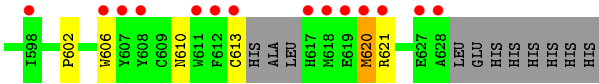
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Nitrous-oxide reductase



• Molecule 1: Nitrous-oxide reductase





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 48.10 – 1.57	Depositor EDS
% Data completeness (in resolution range)	99.3 (100.54-2.14) 97.2 (48.10-1.57)	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 0.255 , 0.253	Depositor DCC
R_{free} test set	6656 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	2.4	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 168776 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.81	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.76	1/4352 (0.0%)	0.89	7/5889 (0.1%)
1	B	0.75	0/4348	0.88	4/5885 (0.1%)
All	All	0.76	1/8700 (0.0%)	0.88	11/11774 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	TRP	CB-CG	-6.86	1.38	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	239	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	268	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	A	123	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	377	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	155	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	268	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	621	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	358	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	B	358	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	530	ARG	NE-CZ-NH1	5.11	122.85	120.30

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	4254	0	4154	31	0
1	B	4243	0	4149	23	0
2	A	50	0	0	1	0
2	B	42	0	0	1	0
All	All	8589	0	8303	54	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 (54) 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: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:167:ILE:N	1:A:167:ILE:HD12	2.27	0.49
1:B:583:VAL:HG13	1:B:595:VAL:HG21	1.95	0.49
1:B:66:TYR:HB2	1:B:83:ILE:HB	1.95	0.49
1:B:434:ASP:O	1:B:435:THR:C	2.51	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:177:ARG:HG3	1:B:238:THR:O	2.17	0.45
1:B:85:SER:HB3	1:B:87:ARG:HG3	1.99	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:176:LEU:HD23	1:B:176:LEU:C	2.39	0.43
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: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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	21	12
1	B	531/636 (84%)	502 (94%)	27 (5%)	2 (0%)	39	33
All	All	1062/1272 (84%)	1007 (95%)	48 (4%)	7 (1%)	26	17

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 ⓘ

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	466/541 (86%)	451 (97%)	15 (3%)	46	44
1	B	466/541 (86%)	457 (98%)	9 (2%)	65	68
All	All	932/1082 (86%)	908 (97%)	24 (3%)	54	54

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	TRP
1	A	193	PHE
1	A	212	ARG
1	A	248	PHE
1	A	270	HIS
1	A	284	LYS
1	A	340	SER
1	A	364	GLU
1	A	510	ASP

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Mol	Chain	Res	Type
1	A	544	PRO
1	A	545	ASN
1	A	586	GLU
1	A	613	CYS
1	A	619	GLU
1	A	621	ARG
1	B	110	LYS
1	B	133	ASP
1	B	230	MET
1	B	410	ASN
1	B	427	THR
1	B	510	ASP
1	B	550	GLU
1	B	613	CYS
1	B	620	MET

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

Mol	Chain	Res	Type
1	A	125	HIS
1	A	126	HIS
1	A	190	ASN
1	A	270	HIS
1	A	321	ASN
1	A	421	GLN
1	A	463	GLN
1	B	128	HIS
1	B	270	HIS
1	B	410	ASN
1	B	419	HIS
1	B	590	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 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 ⓘ

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%)	1.00	67 (12%) 5 8	18, 32, 59, 93	0
1	B	537/636 (84%)	1.06	64 (11%) 6 9	17, 33, 60, 87	0
All	All	1076/1272 (84%)	1.03	131 (12%) 5 8	17, 32, 60, 93	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	TYR	10.3
1	B	292	ASN	7.7
1	A	618	MET	7.1
1	A	212	ARG	6.7
1	B	628	ALA	6.6
1	B	291	TYR	6.5
1	A	612	PHE	5.8
1	B	618	MET	5.6
1	A	292	ASN	5.2
1	B	304	GLY	5.2
1	A	251	CYS	5.0
1	B	517	GLN	4.9
1	A	606	TRP	4.6
1	B	174[A]	HIS	4.4
1	A	252	TYR	4.3
1	B	408	LYS	4.3
1	B	612	PHE	4.3
1	B	470	ASP	4.2
1	B	627	GLU	4.2
1	B	254	SER	4.1
1	A	617	HIS	4.1
1	B	57	VAL	4.1
1	B	293	GLY	4.0
1	A	267	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	193	PHE	4.0
1	B	621	ARG	3.9
1	A	304	GLY	3.9
1	A	619	GLU	3.8
1	B	606	TRP	3.8
1	B	252	TYR	3.7
1	B	289	THR	3.7
1	A	408	LYS	3.5
1	B	531	ASP	3.5
1	A	193	PHE	3.4
1	A	289	THR	3.3
1	B	471	GLU	3.3
1	A	470	ASP	3.2
1	A	291	TYR	3.2
1	A	173	ILE	3.2
1	A	628	ALA	3.1
1	A	458	ARG	3.1
1	B	533	ASN	3.1
1	B	469	GLY	3.0
1	A	549	ASN	3.0
1	A	544	PRO	3.0
1	B	611	TRP	3.0
1	B	295	LYS	3.0
1	B	620	MET	2.9
1	B	608	TYR	2.9
1	B	115	ASP	2.9
1	A	369	LEU	2.9
1	A	602	PRO	2.9
1	A	348	ASP	2.8
1	B	253	ASN	2.8
1	B	315	LYS	2.8
1	A	407	GLU	2.8
1	A	287	LYS	2.7
1	B	251	CYS	2.7
1	B	617	HIS	2.7
1	A	349	ASP	2.7
1	B	468	SER	2.7
1	B	619	GLU	2.7
1	B	62	GLU	2.6
1	B	125	HIS	2.6
1	B	556	GLY	2.6
1	B	532	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	287	LYS	2.6
1	A	254	SER	2.6
1	A	524	MET	2.6
1	A	253	ASN	2.6
1	B	412	LEU	2.5
1	B	58	VAL	2.5
1	B	433	ARG	2.5
1	A	237	ASN	2.5
1	A	555	LEU	2.5
1	B	270	HIS	2.4
1	A	474	LEU	2.4
1	A	627	GLU	2.4
1	B	173	ILE	2.4
1	B	544	PRO	2.4
1	A	59	HIS	2.4
1	B	284	LYS	2.4
1	A	525	ASP	2.4
1	A	294	ASN	2.4
1	A	533	ASN	2.3
1	A	510	ASP	2.3
1	A	295	LYS	2.3
1	B	480	THR	2.3
1	B	311	ILE	2.3
1	A	608	TYR	2.3
1	A	598	ILE	2.3
1	A	620	MET	2.2
1	A	342	VAL	2.2
1	B	70	TRP	2.2
1	A	531	ASP	2.2
1	A	174	HIS	2.2
1	A	288	PHE	2.2
1	A	550	GLU	2.2
1	A	313	VAL	2.2
1	A	236	ASP	2.2
1	A	444	CYS	2.2
1	A	128	HIS	2.2
1	A	546	PHE	2.2
1	B	485	HIS	2.2
1	B	552	LYS	2.2
1	A	410	ASN	2.2
1	B	176	LEU	2.2
1	B	607	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	480	THR	2.2
1	A	171	GLN	2.1
1	B	324	PRO	2.2
1	B	545	ASN	2.1
1	A	485	HIS	2.1
1	B	397	ILE	2.1
1	B	598	ILE	2.1
1	B	352	SER	2.1
1	B	132	THR	2.1
1	A	192	GLU	2.1
1	B	300	ASP	2.1
1	B	389	ASP	2.1
1	B	516	LYS	2.1
1	A	570	GLU	2.1
1	A	284	LYS	2.1
1	A	293	GLY	2.1
1	A	270	HIS	2.0
1	A	481	PHE	2.0
1	A	370	GLY	2.0
1	A	604	VAL	2.0
1	A	571	ASP	2.0
1	B	172	ALA	2.0
1	B	613	CYS	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.