



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:29 AM UTC

PDB ID : 6LR1 / pdb_00006lr1
Title : Hexachlorobenzene Monooxygenase (HcbA1) from Nocardioides sp. strain PD653
Authors : Guo, Y.; Zheng, J.T.; Zhou, N.Y.
Deposited on : 2020-01-15
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

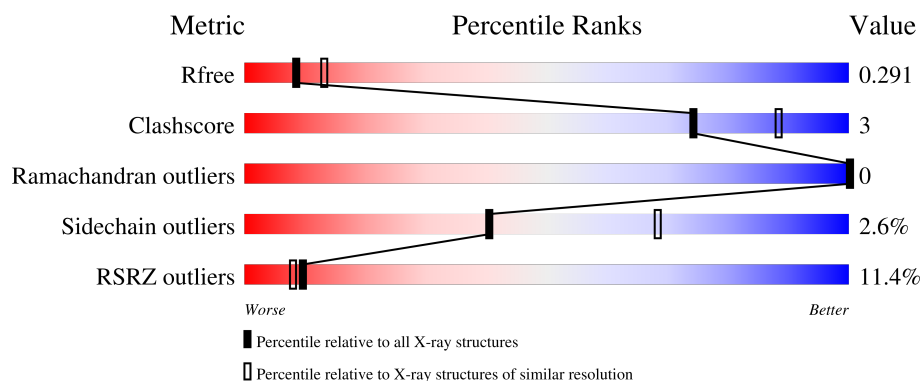
1 Overall quality at a glance

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	451	11% 91% 8%
1	B	451	12% 84% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7138 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 Hexachlorobenzene oxidative dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3529	2219	621	671	18			
1	B	451	Total	C	N	O	S	0	0	0
			3529	2219	621	671	18			

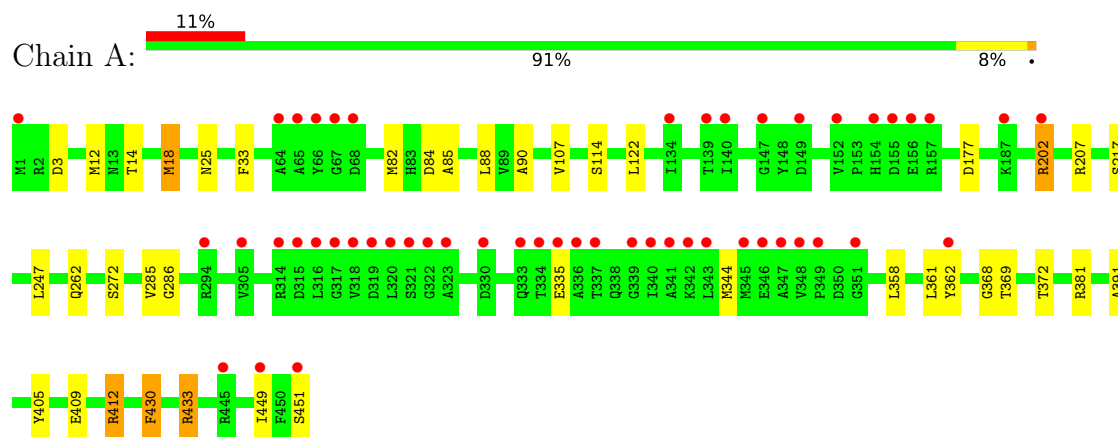
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	37	Total	O	0	0
			37	37		
2	B	43	Total	O	0	0
			43	43		

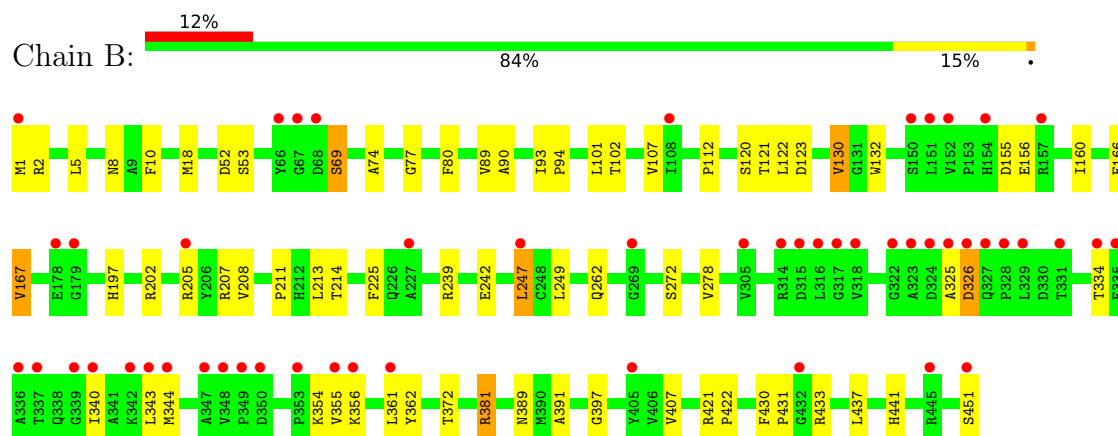
3 Residue-property plots

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: Hexachlorobenzene oxidative dehalogenase



- Molecule 1: Hexachlorobenzene oxidative dehalogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	112.09Å 139.31Å 169.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.33 – 2.50 87.33 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.9 (87.33-2.50) 97.9 (87.33-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.228 , 0.294 0.234 , 0.291	Depositor DCC
R_{free} test set	2236 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtrriage
Anisotropy	0.129	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.41$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7138	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.11 % 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 2.8697e-05. 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	1.12	5/3612 (0.1%)	1.16	14/4898 (0.3%)
1	B	1.23	8/3612 (0.2%)	1.23	12/4898 (0.2%)
All	All	1.18	13/7224 (0.2%)	1.19	26/9796 (0.3%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	THR	C-O	-6.34	1.16	1.23
1	B	132	TRP	C-O	-6.04	1.17	1.24
1	A	202	ARG	C-O	-6.03	1.17	1.24
1	B	130	VAL	C-O	-5.76	1.16	1.24
1	B	166	GLU	CA-C	5.66	1.60	1.52
1	B	213	LEU	C-O	-5.55	1.16	1.24
1	B	208	VAL	C-O	-5.46	1.18	1.24
1	B	121	THR	C-O	-5.21	1.18	1.24
1	B	123	ASP	CA-C	5.18	1.59	1.52
1	A	85	ALA	CA-C	5.18	1.59	1.52
1	A	114	SER	C-O	-5.17	1.18	1.24
1	A	88	LEU	C-O	-5.14	1.18	1.24
1	B	10	PHE	C-O	-5.10	1.17	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	449	ILE	N-CA-C	9.35	122.74	111.05
1	B	433	ARG	N-CA-C	9.26	122.47	110.53
1	A	433	ARG	N-CA-C	8.51	122.09	110.35
1	A	430	PHE	CA-C-N	6.70	128.21	119.84
1	A	430	PHE	C-N-CA	6.70	128.21	119.84
1	B	326	ASP	N-CA-C	6.63	121.08	112.92
1	B	430	PHE	CA-C-N	6.54	128.02	119.84
1	B	430	PHE	C-N-CA	6.54	128.02	119.84
1	B	130	VAL	N-CA-C	6.52	118.08	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	397	GLY	N-CA-C	6.08	120.00	112.64
1	A	217	SER	CA-C-N	-6.03	112.36	119.05
1	A	217	SER	C-N-CA	-6.03	112.36	119.05
1	B	69	SER	N-CA-C	5.92	118.90	109.24
1	A	18	MET	N-CA-C	5.92	121.94	114.31
1	B	407	VAL	N-CA-CB	5.90	114.47	110.52
1	A	33	PHE	N-CA-C	5.82	118.41	111.71
1	A	25	ASN	CA-C-N	5.69	126.07	119.47
1	A	25	ASN	C-N-CA	5.69	126.07	119.47
1	B	242	GLU	N-CA-C	-5.54	106.65	113.41
1	A	405	TYR	N-CA-C	5.50	120.25	112.93
1	B	167	VAL	N-CA-C	5.49	116.12	110.36
1	A	84	ASP	N-CA-C	5.29	118.48	110.64
1	B	74	ALA	N-CA-C	5.27	116.83	111.14
1	A	358	LEU	CA-C-N	-5.21	114.25	119.56
1	A	358	LEU	C-N-CA	-5.21	114.25	119.56
1	B	132	TRP	N-CA-C	5.18	116.84	108.34

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	3529	0	3407	15	0
1	B	3529	0	3407	28	0
2	A	37	0	0	0	0
2	B	43	0	0	0	0
All	All	7138	0	6814	43	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 (43) 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:249:LEU:CD1	1:B:344:MET:HA	2.07	0.85
1:B:247:LEU:HD22	1:B:361:LEU:O	1.90	0.72
1:B:262:GLN:OE1	1:B:272:SER:HB2	1.92	0.69
1:A:430:PHE:HB3	1:A:433:ARG:HD2	1.77	0.65
1:B:326:ASP:O	1:B:354:LYS:HD3	1.98	0.64
1:A:202:ARG:HD2	1:A:207:ARG:NH1	2.14	0.63
1:A:90:ALA:HB2	1:A:122:LEU:HD21	1.81	0.62
1:B:437:LEU:HD13	1:B:441:HIS:ND1	2.19	0.58
1:B:325:ALA:O	1:B:355:VAL:HG22	2.05	0.57
1:B:249:LEU:HD11	1:B:344:MET:HA	1.87	0.54
1:A:202:ARG:HD2	1:A:207:ARG:HH11	1.74	0.53
1:B:90:ALA:HB2	1:B:122:LEU:HD21	1.88	0.53
1:A:3:ASP:O	1:A:381:ARG:NH1	2.42	0.53
1:B:197:HIS:O	1:B:211:PRO:HB3	2.10	0.52
1:B:8:ASN:OD1	1:B:53:SER:OG	2.27	0.51
1:A:262:GLN:OE1	1:A:272:SER:HB2	2.11	0.50
1:B:239:ARG:HG2	1:B:239:ARG:HH11	1.79	0.48
1:A:344:MET:HE2	1:A:361:LEU:HD21	1.94	0.48
1:B:202:ARG:HH21	1:B:207:ARG:HH12	1.61	0.47
1:A:177:ASP:OD2	1:A:451:SER:HB3	2.14	0.47
1:B:249:LEU:HD12	1:B:343:LEU:O	2.15	0.46
1:A:18:MET:HE1	1:A:362:TYR:HB3	1.97	0.45
1:B:112:PRO:CG	1:B:167:VAL:HG11	2.46	0.45
1:B:160:ILE:HG23	1:B:205:ARG:HD3	1.99	0.45
1:B:120:SER:HB2	1:B:214:THR:HG21	1.98	0.44
1:B:18:MET:HE1	1:B:362:TYR:HB3	2.00	0.44
1:B:278:VAL:HG12	1:B:389:ASN:HB2	2.00	0.43
1:A:285:VAL:HA	1:A:368:GLY:O	2.19	0.42
1:B:90:ALA:HB2	1:B:122:LEU:CD2	2.49	0.42
1:A:286:GLY:O	1:A:369:THR:HA	2.19	0.42
1:B:2:ARG:NH2	1:B:52:ASP:OD2	2.53	0.42
1:B:5:LEU:HD21	1:B:381:ARG:HG3	2.01	0.42
1:B:112:PRO:HG2	1:B:167:VAL:HG11	2.00	0.42
1:B:102:THR:HG21	1:B:225:PHE:CE1	2.55	0.42
1:A:18:MET:HE1	1:A:362:TYR:CB	2.50	0.41
1:B:77:GLY:HA2	1:B:80:PHE:O	2.21	0.41
1:A:18:MET:HG3	1:A:391:ALA:HB1	2.02	0.41
1:A:409:GLU:OE1	1:A:412:ARG:NH2	2.41	0.41
1:B:18:MET:HG3	1:B:391:ALA:HB1	2.03	0.40
1:B:89:VAL:HG13	1:B:101:LEU:HB3	2.03	0.40
1:B:421:ARG:HD2	1:B:422:PRO:HD2	2.04	0.40
1:A:12:MET:HE2	1:A:82:MET:CE	2.50	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ILE:HB	1:B:94:PRO:HD3	2.02	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	449/451 (100%)	429 (96%)	20 (4%)	0	100	100
1	B	449/451 (100%)	432 (96%)	17 (4%)	0	100	100
All	All	898/902 (100%)	861 (96%)	37 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	366/366 (100%)	361 (99%)	5 (1%)	59	81
1	B	366/366 (100%)	352 (96%)	14 (4%)	29	56
All	All	732/732 (100%)	713 (97%)	19 (3%)	40	68

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	VAL
1	A	247	LEU
1	A	335	GLU
1	A	372	THR
1	A	412	ARG
1	B	1	MET
1	B	69	SER
1	B	107	VAL
1	B	130	VAL
1	B	155	ASP
1	B	156	GLU
1	B	247	LEU
1	B	334	THR
1	B	340	ILE
1	B	356	LYS
1	B	372	THR
1	B	381	ARG
1	B	431	PRO
1	B	451	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	76	GLN
1	A	133	ASN
1	A	301	GLN
1	A	327	GLN
1	A	338	GLN
1	B	76	GLN
1	B	133	ASN
1	B	144	GLN

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	451/451 (100%)	0.47	51 (11%) 10 8	21, 36, 82, 117	0
1	B	451/451 (100%)	0.64	52 (11%) 9 8	22, 36, 78, 102	0
All	All	902/902 (100%)	0.56	103 (11%) 10 8	21, 36, 80, 117	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.8
1	B	1	MET	6.5
1	A	66	TYR	5.8
1	A	152	VAL	5.8
1	B	349	PRO	5.1
1	B	355	VAL	5.1
1	B	325	ALA	4.8
1	B	323	ALA	4.8
1	A	348	VAL	4.7
1	A	349	PRO	4.7
1	A	345	MET	4.7
1	B	343	LEU	4.5
1	A	322	GLY	4.5
1	B	361	LEU	4.5
1	A	316	LEU	4.3
1	A	155	ASP	4.2
1	A	343	LEU	4.2
1	B	353	PRO	4.0
1	B	356	LYS	4.0
1	A	314	ARG	4.0
1	B	67	GLY	3.9
1	B	340	ILE	3.7
1	B	316	LEU	3.6
1	B	336	ALA	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	154	HIS	3.6
1	B	344	MET	3.6
1	A	342	LYS	3.5
1	A	319	ASP	3.5
1	B	348	VAL	3.5
1	A	317	GLY	3.5
1	B	322	GLY	3.4
1	B	324	ASP	3.4
1	A	445	ARG	3.3
1	B	152	VAL	3.3
1	A	318	VAL	3.3
1	B	328	PRO	3.2
1	A	67	GLY	3.2
1	A	187	LYS	3.2
1	A	320	LEU	3.2
1	B	68	ASP	3.1
1	B	157	ARG	3.1
1	B	337	THR	3.0
1	B	335	GLU	3.0
1	A	294	ARG	3.0
1	A	347	ALA	2.9
1	B	347	ALA	2.9
1	B	326	ASP	2.9
1	A	451	SER	2.9
1	B	314	ARG	2.9
1	B	445	ARG	2.9
1	A	333	GLN	2.9
1	B	178	GLU	2.9
1	B	205	ARG	2.8
1	B	451	SER	2.8
1	A	336	ALA	2.8
1	A	321	SER	2.8
1	A	340	ILE	2.7
1	A	202	ARG	2.7
1	A	337	THR	2.7
1	B	331	THR	2.7
1	B	269	GLY	2.6
1	B	108	ILE	2.6
1	B	66	TYR	2.6
1	A	64	ALA	2.6
1	B	339	GLY	2.6
1	A	157	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	334	THR	2.6
1	B	405	TYR	2.6
1	A	139	THR	2.6
1	B	227	ALA	2.6
1	A	315	ASP	2.5
1	A	65	ALA	2.5
1	A	156	GLU	2.5
1	A	341	ALA	2.4
1	A	351	GLY	2.4
1	A	305	VAL	2.4
1	A	449	ILE	2.4
1	A	330	ASP	2.4
1	B	247	LEU	2.4
1	B	305	VAL	2.4
1	B	318	VAL	2.4
1	B	315	ASP	2.3
1	B	327	GLN	2.3
1	A	335	GLU	2.3
1	B	329	LEU	2.3
1	B	350	ASP	2.3
1	A	147	GLY	2.2
1	B	150	SER	2.2
1	B	151	LEU	2.2
1	B	179	GLY	2.2
1	A	140	ILE	2.2
1	A	346	GLU	2.2
1	B	342	LYS	2.2
1	B	154	HIS	2.2
1	A	334	THR	2.2
1	B	432	GLY	2.2
1	A	323	ALA	2.1
1	B	317	GLY	2.1
1	A	362	TYR	2.1
1	A	339	GLY	2.0
1	A	134	ILE	2.0
1	A	68	ASP	2.0
1	A	149	ASP	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.