



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:07 PM GMT

PDB ID : 2DH1
Title : Crystal structure of peanut lectin lactose-azobenzene-4,4'-dicarboxylic acid-lactose complex
Authors : Natchiar, S.K.; Srinivas, O.; Nivedita, M.; Sagarika, D.; Jayaraman, N.; Suro-
lia, A.; Vijayan, M.
Deposited on : 2006-03-17
Resolution : 7.65 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

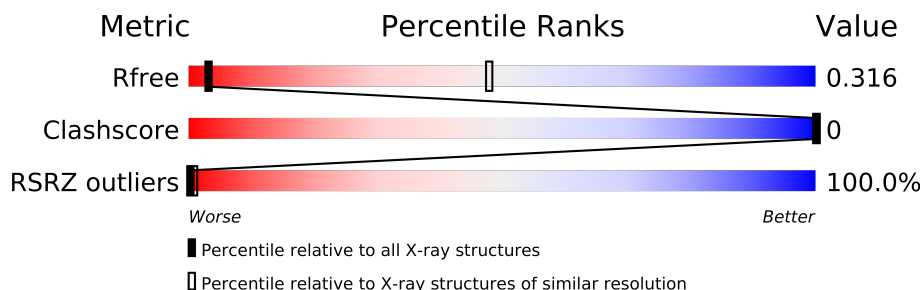
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 7.65 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}	66092	1106 (11.50-3.50)
Clashscore	79885	1006 (11.50-3.54)
RSRZ outliers	66119	1105 (11.50-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	236	
1	B	236	
1	C	236	
1	D	236	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 928 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

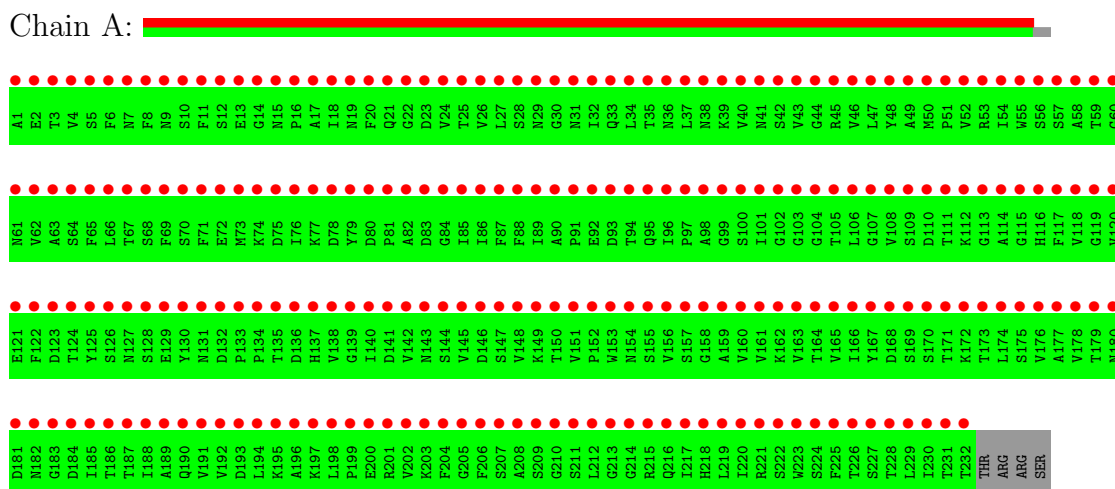
- Molecule 1 is a protein called Galactose-binding lectin.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	232	Total 232	C 232	0	0	232
1	B	232	Total 232	C 232	0	0	232
1	C	232	Total 232	C 232	0	0	232
1	D	232	Total 232	C 232	0	0	232

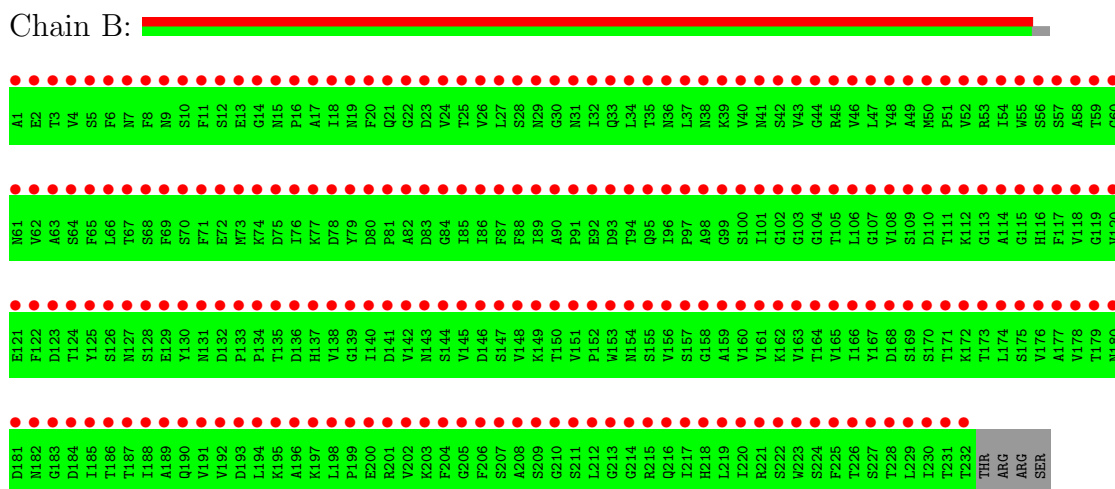
3 Residue-property plots

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.

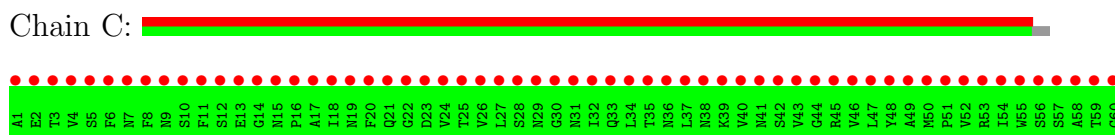
- Molecule 1: Galactose-binding lectin

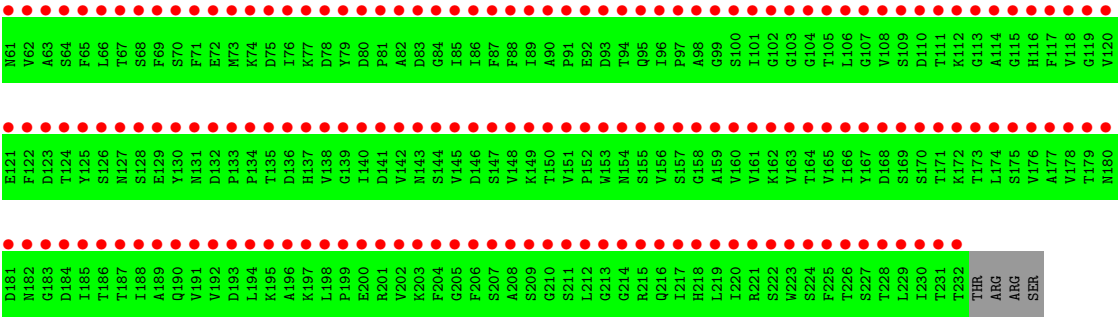


- Molecule 1: Galactose-binding lectin



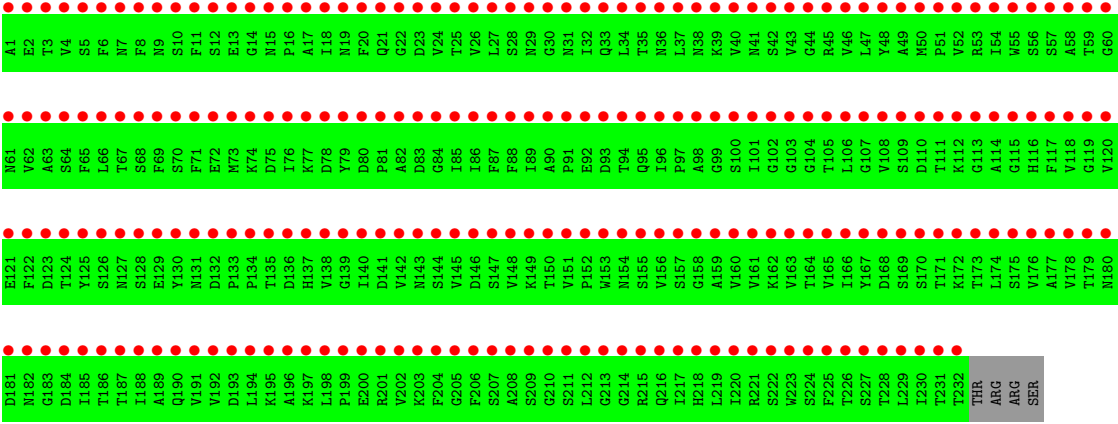
- Molecule 1: Galactose-binding lectin





● Molecule 1: Galactose-binding lectin

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	92.75Å 92.75Å 473.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 7.65 19.99 – 7.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-7.65) 99.7 (19.99-7.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.42 (at 7.78Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.355 , 0.377 0.361 , 0.316	Depositor DCC
R_{free} test set	104 reflections (4.78%)	DCC
Wilson B-factor (Å ²)	390.9	Xtriage
Anisotropy	0.950	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.88 , 95.2	EDS
Estimated twinning fraction	0.458 for -h,k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 2271 reflections	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	928	wwPDB-VP
Average B, all atoms (Å ²)	347.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	$\# Z > 5$

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	232	0	0	0	0
1	B	232	0	0	0	0
1	C	232	0	0	0	0
1	D	232	0	0	0	0
All	All	928	0	0	0	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	232/236 (98%)	44.48	232 (100%) 0 1	316, 343, 362, 369	0
1	B	232/236 (98%)	43.25	232 (100%) 0 1	314, 343, 360, 368	0
1	C	232/236 (98%)	42.60	232 (100%) 0 1	321, 354, 371, 375	0
1	D	232/236 (98%)	43.44	232 (100%) 0 1	322, 352, 373, 381	0
All	All	928/944 (98%)	43.44	928 (100%) 0 1	314, 349, 368, 381	0

All (928) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	31	ASN	140.1
1	C	109	SER	135.0
1	B	27	LEU	118.5
1	B	189	ALA	118.2
1	B	30	GLY	117.6
1	C	136	ASP	112.3
1	A	71	PHE	110.5
1	C	107	GLY	108.1
1	C	208	ALA	106.9
1	B	175	SER	106.7
1	A	34	LEU	103.5
1	C	203	LYS	103.3
1	D	152	PRO	100.6
1	C	105	THR	100.0
1	A	33	GLN	97.8
1	D	201	ARG	97.1
1	C	201	ARG	97.1
1	D	202	VAL	96.3
1	D	203	LYS	95.7
1	C	97	PRO	95.3
1	C	115	GLY	93.4

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Mol	Chain	Res	Type	RSRZ
1	C	106	LEU	93.3
1	A	167	TYR	92.8
1	B	40	VAL	89.5
1	C	110	ASP	88.9
1	A	23	ASP	87.4
1	C	202	VAL	86.2
1	A	42	SER	85.9
1	D	229	LEU	84.8
1	A	220	ILE	84.3
1	D	92	GLU	84.0
1	A	13	GLU	82.8
1	A	203	LYS	82.6
1	C	114	ALA	82.0
1	D	51	PRO	81.9
1	D	110	ASP	81.8
1	B	39	LYS	80.7
1	C	99	GLY	79.7
1	D	35	THR	78.9
1	B	219	LEU	78.7
1	B	109	SER	78.4
1	D	136	ASP	78.3
1	C	209	SER	77.9
1	A	136	ASP	77.9
1	D	109	SER	77.7
1	B	49	ALA	77.6
1	A	92	GLU	77.2
1	A	26	VAL	76.8
1	B	42	SER	76.8
1	D	75	ASP	76.4
1	C	174	LEU	76.3
1	A	72	GLU	76.3
1	B	34	LEU	76.3
1	A	159	ALA	76.2
1	B	23	ASP	75.8
1	A	86	ILE	75.4
1	A	49	ALA	74.9
1	C	86	ILE	74.9
1	B	203	LYS	74.3
1	B	2	GLU	73.9
1	D	105	THR	73.8
1	B	53	ARG	73.6
1	D	74	LYS	73.5

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Mol	Chain	Res	Type	RSRZ
1	B	92	GLU	72.5
1	B	152	PRO	72.4
1	C	35	THR	72.1
1	A	174	LEU	71.5
1	B	22	GLY	71.3
1	D	162	LYS	70.0
1	A	165	VAL	69.9
1	D	221	ARG	69.8
1	D	97	PRO	69.7
1	D	98	ALA	69.6
1	B	10	SER	69.4
1	D	99	GLY	69.2
1	A	166	ILE	69.0
1	A	87	PHE	68.9
1	B	32	ILE	68.7
1	D	34	LEU	68.2
1	B	201	ARG	68.1
1	A	219	LEU	68.0
1	C	98	ALA	67.9
1	D	164	THR	67.7
1	B	174	LEU	67.3
1	A	41	ASN	67.2
1	C	121	GLU	67.0
1	C	175	SER	66.8
1	A	121	GLU	66.2
1	A	202	VAL	66.1
1	D	23	ASP	65.9
1	A	183	GLY	65.8
1	A	137	HIS	65.7
1	B	202	VAL	65.7
1	C	224	SER	65.4
1	D	230	ILE	65.4
1	B	167	TYR	65.2
1	B	182	ASN	65.0
1	D	165	VAL	65.0
1	A	155	SER	64.7
1	D	115	GLY	64.6
1	D	208	ALA	64.0
1	C	207	SER	63.9
1	D	69	PHE	63.9
1	C	165	VAL	63.6
1	A	48	TYR	63.4

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Mol	Chain	Res	Type	RSRZ
1	A	21	GLN	63.2
1	D	204	PHE	63.1
1	B	153	TRP	63.1
1	D	39	LYS	63.0
1	D	215	ARG	62.9
1	C	16	PRO	62.9
1	A	208	ALA	62.9
1	A	156	VAL	62.9
1	A	73	MET	62.9
1	B	55	TRP	62.8
1	A	27	LEU	62.7
1	B	26	VAL	62.7
1	B	141	ASP	62.7
1	D	67	THR	62.4
1	D	223	TRP	62.4
1	D	137	HIS	62.4
1	A	173	THR	62.3
1	B	176	VAL	62.3
1	C	204	PHE	62.2
1	B	229	LEU	62.0
1	B	130	TYR	61.9
1	C	7	ASN	61.6
1	C	89	ILE	61.5
1	D	224	SER	61.5
1	A	97	PRO	61.4
1	C	6	PHE	61.2
1	D	44	GLY	61.1
1	D	50	MET	61.1
1	A	195	LYS	60.9
1	D	107	GLY	60.9
1	A	39	LYS	60.9
1	C	88	PHE	60.7
1	B	33	GLN	60.6
1	A	175	SER	60.6
1	B	50	MET	60.4
1	D	166	ILE	60.4
1	B	154	ASN	60.4
1	A	40	VAL	60.3
1	D	17	ALA	60.2
1	A	226	THR	60.1
1	C	51	PRO	60.0
1	A	80	ASP	60.0

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Mol	Chain	Res	Type	RSRZ
1	A	210	GLY	59.9
1	A	141	ASP	59.8
1	C	85	ILE	59.8
1	C	43	VAL	59.7
1	A	93	ASP	59.5
1	A	32	ILE	59.4
1	B	220	ILE	59.3
1	D	163	VAL	59.0
1	B	81	PRO	58.7
1	D	121	GLU	58.7
1	C	123	ASP	58.5
1	A	31	ASN	58.3
1	D	231	THR	58.2
1	D	153	TRP	58.2
1	D	207	SER	58.1
1	D	228	THR	58.1
1	D	33	GLN	58.1
1	D	81	PRO	58.1
1	D	175	SER	58.0
1	D	49	ALA	58.0
1	D	68	SER	58.0
1	A	53	ARG	57.9
1	A	76	ILE	57.8
1	A	35	THR	57.8
1	C	167	TYR	57.8
1	B	52	VAL	57.7
1	A	153	TRP	57.6
1	C	22	GLY	57.6
1	A	160	VAL	57.5
1	A	30	GLY	57.4
1	B	41	ASN	57.4
1	C	48	TYR	57.3
1	B	97	PRO	57.3
1	C	116	HIS	57.1
1	B	99	GLY	57.1
1	D	45	ARG	57.0
1	D	86	ILE	57.0
1	D	19	ASN	56.9
1	B	3	THR	56.8
1	A	164	THR	56.8
1	C	81	PRO	56.8
1	B	159	ALA	56.7

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Mol	Chain	Res	Type	RSRZ
1	D	131	ASN	56.7
1	B	140	ILE	56.4
1	B	72	GLU	56.3
1	D	52	VAL	56.2
1	A	163	VAL	56.1
1	A	8	PHE	56.1
1	B	71	PHE	56.0
1	A	77	LYS	56.0
1	C	82	ALA	55.7
1	B	194	LEU	55.5
1	D	193	ASP	55.2
1	D	196	ALA	55.2
1	D	41	ASN	55.2
1	A	206	PHE	55.2
1	D	222	SER	55.1
1	C	44	GLY	55.0
1	C	173	THR	54.9
1	D	216	GLN	54.8
1	D	16	PRO	54.8
1	A	230	ILE	54.8
1	B	221	ARG	54.8
1	B	210	GLY	54.7
1	D	102	GLY	54.5
1	B	91	PRO	54.4
1	B	48	TYR	54.4
1	A	50	MET	54.3
1	A	29	ASN	54.3
1	A	10	SER	54.1
1	A	19	ASN	54.1
1	B	208	ALA	54.0
1	C	96	ILE	54.0
1	A	201	ARG	54.0
1	C	153	TRP	53.9
1	C	83	ASP	53.9
1	B	21	GLN	53.8
1	C	17	ALA	53.7
1	A	89	ILE	53.7
1	A	180	ASN	53.7
1	B	44	GLY	53.3
1	A	150	THR	53.3
1	C	147	SER	53.0
1	B	18	ILE	52.9

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Mol	Chain	Res	Type	RSRZ
1	C	30	GLY	52.6
1	D	176	VAL	52.6
1	C	125	TYR	52.5
1	A	154	ASN	52.4
1	D	42	SER	52.4
1	C	137	HIS	52.4
1	B	181	ASP	52.3
1	A	61	ASN	52.2
1	C	172	LYS	52.1
1	A	91	PRO	52.1
1	A	218	HIS	52.1
1	B	77	LYS	51.7
1	C	122	PHE	51.7
1	D	48	TYR	51.7
1	C	200	GLU	51.6
1	B	79	TYR	51.6
1	B	8	PHE	51.6
1	B	73	MET	51.1
1	C	69	PHE	51.1
1	A	229	LEU	51.0
1	A	214	GLY	50.9
1	A	70	SER	50.9
1	A	228	THR	50.9
1	C	216	GLN	50.9
1	D	205	GLY	50.8
1	B	190	GLN	50.7
1	C	223	TRP	50.6
1	B	183	GLY	50.5
1	A	85	ILE	50.4
1	C	47	LEU	50.4
1	B	156	VAL	50.4
1	C	228	THR	50.3
1	D	116	HIS	50.3
1	A	221	ARG	50.3
1	B	173	THR	50.3
1	C	74	LYS	50.1
1	C	49	ALA	50.0
1	C	21	GLN	50.0
1	A	207	SER	49.9
1	B	87	PHE	49.8
1	C	220	ILE	49.8
1	C	141	ASP	49.8

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Mol	Chain	Res	Type	RSRZ
1	B	86	ILE	49.7
1	B	16	PRO	49.7
1	D	30	GLY	49.7
1	D	22	GLY	49.6
1	B	57	SER	49.6
1	A	18	ILE	49.6
1	B	105	THR	49.3
1	B	218	HIS	49.3
1	A	69	PHE	49.0
1	C	164	THR	49.0
1	C	108	VAL	48.9
1	B	151	VAL	48.9
1	C	205	GLY	48.9
1	C	128	SER	48.6
1	B	80	ASP	48.5
1	B	36	ASN	48.5
1	B	9	ASN	48.5
1	D	93	ASP	48.4
1	B	98	ALA	48.4
1	A	20	PHE	48.3
1	D	113	GLY	48.2
1	A	15	ASN	48.2
1	A	68	SER	48.1
1	D	87	PHE	48.1
1	C	92	GLU	47.8
1	D	180	ASN	47.8
1	B	206	PHE	47.7
1	D	190	GLN	47.6
1	C	94	THR	47.5
1	D	37	LEU	47.4
1	D	106	LEU	47.4
1	A	172	LYS	47.4
1	B	108	VAL	47.4
1	D	27	LEU	47.3
1	A	78	ASP	47.3
1	D	174	LEU	47.2
1	D	66	LEU	47.1
1	B	164	THR	47.1
1	B	200	GLU	47.1
1	A	6	PHE	47.1
1	D	89	ILE	47.0
1	D	103	GLY	47.0

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Mol	Chain	Res	Type	RSRZ
1	C	176	VAL	46.9
1	D	47	LEU	46.9
1	D	91	PRO	46.9
1	D	104	GLY	46.9
1	C	192	VAL	46.9
1	A	3	THR	46.9
1	B	142	VAL	46.8
1	B	38	ASN	46.8
1	D	154	ASN	46.7
1	D	140	ILE	46.7
1	B	155	SER	46.7
1	A	211	SER	46.6
1	C	166	ILE	46.6
1	C	58	ALA	46.5
1	D	226	THR	46.5
1	C	91	PRO	46.4
1	D	82	ALA	46.3
1	B	14	GLY	46.3
1	A	12	SER	46.2
1	A	5	SER	46.2
1	D	192	VAL	46.1
1	B	24	VAL	46.1
1	C	75	ASP	46.1
1	B	25	THR	46.1
1	B	85	ILE	46.0
1	B	146	ASP	46.0
1	C	68	SER	46.0
1	A	223	TRP	45.9
1	B	196	ALA	45.9
1	D	177	ALA	45.9
1	D	76	ILE	45.8
1	D	212	LEU	45.8
1	D	211	SER	45.7
1	A	43	VAL	45.7
1	A	14	GLY	45.5
1	C	196	ALA	45.3
1	B	29	ASN	45.3
1	C	206	PHE	45.3
1	D	214	GLY	45.2
1	B	83	ASP	45.2
1	A	193	ASP	45.1
1	A	9	ASN	45.1

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Mol	Chain	Res	Type	RSRZ
1	D	88	PHE	45.1
1	C	102	GLY	45.1
1	A	44	GLY	45.1
1	D	178	VAL	45.1
1	B	172	LYS	45.0
1	D	96	ILE	45.0
1	B	70	SER	44.9
1	C	142	VAL	44.8
1	A	88	PHE	44.8
1	B	13	GLU	44.7
1	B	163	VAL	44.7
1	A	176	VAL	44.5
1	D	200	GLU	44.5
1	A	24	VAL	44.5
1	D	148	VAL	44.4
1	D	124	THR	44.3
1	D	101	ILE	44.3
1	D	147	SER	44.3
1	D	150	THR	44.2
1	C	129	GLU	44.2
1	A	184	ASP	44.1
1	B	35	THR	44.1
1	A	110	ASP	44.0
1	D	90	ALA	44.0
1	A	38	ASN	44.0
1	C	191	VAL	44.0
1	B	158	GLY	43.9
1	A	215	ARG	43.7
1	B	15	ASN	43.6
1	C	67	THR	43.6
1	D	24	VAL	43.6
1	C	144	SER	43.6
1	C	210	GLY	43.6
1	B	193	ASP	43.6
1	C	70	SER	43.4
1	B	37	LEU	43.4
1	B	116	HIS	43.3
1	C	90	ALA	43.3
1	C	190	GLN	43.3
1	D	7	ASN	43.3
1	A	17	ALA	43.3
1	A	197	LYS	43.3

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Mol	Chain	Res	Type	RSRZ
1	A	36	ASN	43.3
1	A	62	VAL	43.2
1	A	196	ALA	43.2
1	D	80	ASP	43.1
1	C	183	GLY	43.0
1	A	117	PHE	43.0
1	A	7	ASN	42.9
1	D	43	VAL	42.9
1	C	189	ALA	42.8
1	D	206	PHE	42.8
1	B	51	PRO	42.8
1	A	67	THR	42.8
1	D	13	GLU	42.7
1	D	220	ILE	42.5
1	D	218	HIS	42.5
1	C	100	SER	42.4
1	C	226	THR	42.3
1	C	221	ARG	42.3
1	B	47	LEU	42.2
1	A	122	PHE	42.2
1	A	168	ASP	42.2
1	C	39	LYS	42.2
1	D	149	LYS	42.1
1	C	215	ARG	42.1
1	D	79	TYR	42.1
1	A	140	ILE	42.0
1	C	193	ASP	42.0
1	A	90	ALA	41.9
1	C	179	THR	41.9
1	C	23	ASP	41.9
1	D	72	GLU	41.9
1	A	16	PRO	41.8
1	D	21	GLN	41.8
1	D	70	SER	41.7
1	C	45	ARG	41.5
1	A	133	PRO	41.5
1	A	83	ASP	41.4
1	B	11	PHE	41.2
1	C	5	SER	41.2
1	D	210	GLY	41.2
1	D	73	MET	41.2
1	B	110	ASP	41.1

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Mol	Chain	Res	Type	RSRZ
1	C	37	LEU	41.1
1	A	98	ALA	41.1
1	C	180	ASN	41.1
1	B	93	ASP	41.0
1	C	84	GLY	41.0
1	D	14	GLY	40.9
1	B	209	SER	40.8
1	B	121	GLU	40.8
1	B	101	ILE	40.7
1	D	83	ASP	40.7
1	C	120	VAL	40.7
1	A	189	ALA	40.7
1	B	223	TRP	40.7
1	D	187	THR	40.7
1	C	34	LEU	40.6
1	C	124	THR	40.6
1	B	228	THR	40.6
1	C	53	ARG	40.6
1	D	173	THR	40.6
1	C	50	MET	40.6
1	A	224	SER	40.6
1	C	104	GLY	40.6
1	B	214	GLY	40.5
1	A	111	THR	40.4
1	C	101	ILE	40.3
1	A	151	VAL	40.3
1	D	10	SER	40.3
1	A	152	PRO	40.2
1	C	139	GLY	40.1
1	B	69	PHE	40.1
1	C	171	THR	40.0
1	B	157	SER	40.0
1	C	87	PHE	40.0
1	C	229	LEU	39.9
1	B	61	ASN	39.9
1	A	74	LYS	39.7
1	C	18	ILE	39.7
1	A	158	GLY	39.6
1	B	76	ILE	39.5
1	A	222	SER	39.5
1	D	18	ILE	39.5
1	C	59	THR	39.4

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Mol	Chain	Res	Type	RSRZ
1	A	79	TYR	39.4
1	A	45	ARG	39.4
1	A	227	SER	39.3
1	C	163	VAL	39.2
1	D	179	THR	39.2
1	B	160	VAL	39.1
1	B	215	ARG	39.1
1	D	25	THR	39.1
1	A	146	ASP	39.1
1	B	62	VAL	39.0
1	C	71	PHE	39.0
1	B	168	ASP	38.8
1	C	111	THR	38.8
1	A	82	ALA	38.8
1	B	103	GLY	38.7
1	B	28	SER	38.7
1	D	11	PHE	38.7
1	B	143	ASN	38.6
1	C	143	ASN	38.6
1	D	227	SER	38.6
1	D	125	TYR	38.6
1	A	99	GLY	38.6
1	C	162	LYS	38.6
1	C	184	ASP	38.5
1	B	192	VAL	38.5
1	A	225	PHE	38.5
1	C	117	PHE	38.5
1	D	183	GLY	38.5
1	B	43	VAL	38.3
1	C	19	ASN	38.3
1	D	172	LYS	38.3
1	C	25	THR	38.2
1	C	230	ILE	38.2
1	C	15	ASN	38.2
1	D	185	ILE	38.2
1	B	171	THR	38.1
1	D	58	ALA	38.1
1	C	214	GLY	38.0
1	D	128	SER	38.0
1	A	84	GLY	38.0
1	D	127	ASN	38.0
1	C	227	SER	37.9

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Mol	Chain	Res	Type	RSRZ
1	D	85	ILE	37.9
1	B	12	SER	37.8
1	A	120	VAL	37.8
1	C	131	ASN	37.8
1	A	75	ASP	37.7
1	D	167	TYR	37.7
1	A	55	TRP	37.7
1	D	130	TYR	37.6
1	B	60	GLY	37.6
1	B	102	GLY	37.6
1	B	226	THR	37.6
1	B	222	SER	37.5
1	C	113	GLY	37.5
1	A	103	GLY	37.5
1	A	212	LEU	37.4
1	D	181	ASP	37.4
1	A	37	LEU	37.4
1	D	65	PHE	37.3
1	C	63	ALA	37.2
1	C	10	SER	37.2
1	B	204	PHE	37.2
1	A	105	THR	37.1
1	A	109	SER	37.1
1	A	135	THR	37.0
1	D	225	PHE	37.0
1	B	66	LEU	36.9
1	D	161	VAL	36.8
1	B	111	THR	36.6
1	C	222	SER	36.6
1	D	100	SER	36.6
1	D	53	ARG	36.5
1	A	190	GLN	36.5
1	A	147	SER	36.4
1	D	15	ASN	36.4
1	D	191	VAL	36.4
1	B	165	VAL	36.3
1	A	209	SER	36.3
1	A	157	SER	36.3
1	D	209	SER	36.1
1	D	219	LEU	36.1
1	A	100	SER	36.1
1	A	2	GLU	36.1

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Mol	Chain	Res	Type	RSRZ
1	C	168	ASP	36.0
1	B	89	ILE	36.0
1	B	100	SER	36.0
1	A	188	ILE	36.0
1	A	142	VAL	36.0
1	B	17	ALA	35.8
1	D	94	THR	35.8
1	A	101	ILE	35.8
1	C	76	ILE	35.7
1	D	189	ALA	35.7
1	D	3	THR	35.6
1	B	162	LYS	35.6
1	A	194	LEU	35.5
1	B	56	SER	35.5
1	C	42	SER	35.5
1	A	143	ASN	35.4
1	D	217	ILE	35.4
1	B	67	THR	35.3
1	C	170	SER	35.3
1	A	161	VAL	35.3
1	A	52	VAL	35.2
1	B	195	LYS	35.1
1	A	81	PRO	35.1
1	A	66	LEU	35.1
1	C	225	PHE	35.0
1	C	169	SER	35.0
1	D	122	PHE	35.0
1	B	1	ALA	35.0
1	A	139	GLY	34.9
1	A	60	GLY	34.9
1	C	152	PRO	34.8
1	D	9	ASN	34.7
1	A	169	SER	34.7
1	B	188	ILE	34.6
1	D	195	LYS	34.6
1	A	118	VAL	34.5
1	B	136	ASP	34.5
1	C	12	SER	34.5
1	A	162	LYS	34.5
1	C	188	ILE	34.5
1	A	22	GLY	34.5
1	B	88	PHE	34.4

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Mol	Chain	Res	Type	RSRZ
1	B	106	LEU	34.4
1	C	149	LYS	34.3
1	B	19	ASN	34.3
1	B	131	ASN	34.3
1	C	9	ASN	34.2
1	A	51	PRO	34.2
1	A	132	ASP	34.2
1	B	137	HIS	34.2
1	C	127	ASN	34.2
1	B	184	ASP	34.2
1	D	31	ASN	34.1
1	C	65	PHE	34.1
1	C	41	ASN	34.0
1	C	36	ASN	34.0
1	B	187	THR	33.9
1	C	119	GLY	33.8
1	D	114	ALA	33.8
1	A	47	LEU	33.8
1	A	145	VAL	33.8
1	C	130	TYR	33.7
1	D	186	THR	33.7
1	A	58	ALA	33.6
1	D	63	ALA	33.5
1	B	145	VAL	33.5
1	D	108	VAL	33.5
1	B	84	GLY	33.5
1	B	207	SER	33.5
1	A	198	LEU	33.4
1	D	55	TRP	33.4
1	A	192	VAL	33.3
1	D	12	SER	33.3
1	A	119	GLY	33.2
1	C	150	THR	33.2
1	C	118	VAL	33.2
1	B	7	ASN	33.2
1	D	182	ASN	33.1
1	D	6	PHE	33.1
1	D	8	PHE	33.1
1	C	133	PRO	32.9
1	B	169	SER	32.9
1	D	129	GLU	32.8
1	C	40	VAL	32.8

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Mol	Chain	Res	Type	RSRZ
1	B	78	ASP	32.7
1	C	148	VAL	32.7
1	D	84	GLY	32.6
1	C	177	ALA	32.6
1	A	204	PHE	32.6
1	A	179	THR	32.6
1	B	82	ALA	32.6
1	B	161	VAL	32.6
1	C	195	LYS	32.5
1	C	13	GLU	32.5
1	D	2	GLU	32.4
1	D	20	PHE	32.3
1	C	11	PHE	32.3
1	D	28	SER	32.3
1	D	36	ASN	32.3
1	B	4	VAL	32.2
1	C	161	VAL	32.2
1	B	112	LYS	32.1
1	B	177	ALA	32.0
1	A	116	HIS	32.0
1	C	93	ASP	32.0
1	B	144	SER	32.0
1	B	227	SER	32.0
1	A	181	ASP	31.9
1	B	129	GLU	31.9
1	B	147	SER	31.9
1	D	64	SER	31.9
1	D	139	GLY	31.8
1	A	191	VAL	31.7
1	C	80	ASP	31.7
1	A	124	THR	31.7
1	A	200	GLU	31.6
1	D	138	VAL	31.6
1	D	111	THR	31.5
1	C	218	HIS	31.5
1	A	46	VAL	31.5
1	A	25	THR	31.5
1	C	62	VAL	31.2
1	B	166	ILE	31.1
1	A	104	GLY	31.0
1	A	65	PHE	31.0
1	C	212	LEU	30.9

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Mol	Chain	Res	Type	RSRZ
1	A	94	THR	30.9
1	A	138	VAL	30.9
1	C	8	PHE	30.9
1	C	181	ASP	30.8
1	D	40	VAL	30.8
1	A	102	GLY	30.7
1	C	154	ASN	30.6
1	B	230	ILE	30.5
1	C	103	GLY	30.4
1	C	185	ILE	30.4
1	C	54	ILE	30.3
1	A	149	LYS	30.3
1	D	59	THR	30.3
1	C	146	ASP	30.3
1	B	180	ASN	30.2
1	A	95	GLN	30.2
1	D	168	ASP	30.2
1	B	135	THR	30.2
1	C	134	PRO	30.2
1	B	117	PHE	30.2
1	C	126	SER	30.2
1	A	187	THR	30.2
1	C	27	LEU	30.1
1	D	151	VAL	29.9
1	B	90	ALA	29.7
1	C	135	THR	29.6
1	D	146	ASP	29.6
1	D	120	VAL	29.6
1	B	45	ARG	29.6
1	B	224	SER	29.6
1	B	139	GLY	29.4
1	B	211	SER	29.4
1	C	3	THR	29.4
1	A	171	THR	29.3
1	C	199	PRO	29.3
1	D	117	PHE	29.3
1	D	171	THR	29.2
1	B	63	ALA	28.9
1	C	2	GLU	28.9
1	D	144	SER	28.9
1	D	141	ASP	28.9
1	B	122	PHE	28.6

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Mol	Chain	Res	Type	RSRZ
1	C	217	ILE	28.6
1	C	79	TYR	28.6
1	B	132	ASP	28.6
1	A	186	THR	28.5
1	C	178	VAL	28.5
1	A	59	THR	28.4
1	C	138	VAL	28.4
1	D	213	GLY	28.4
1	A	1	ALA	28.4
1	C	20	PHE	28.3
1	C	95	GLN	28.3
1	B	150	THR	28.2
1	A	64	SER	28.1
1	C	132	ASP	28.0
1	B	58	ALA	28.0
1	D	5	SER	27.9
1	C	73	MET	27.7
1	C	33	GLN	27.7
1	D	56	SER	27.7
1	D	184	ASP	27.6
1	B	199	PRO	27.6
1	D	71	PHE	27.6
1	D	197	LYS	27.4
1	A	11	PHE	27.3
1	C	182	ASN	27.3
1	C	31	ASN	27.3
1	D	188	ILE	27.2
1	D	57	SER	27.2
1	C	60	GLY	27.1
1	A	56	SER	27.1
1	A	115	GLY	27.1
1	D	199	PRO	27.0
1	A	199	PRO	26.9
1	A	112	LYS	26.9
1	A	144	SER	26.8
1	D	126	SER	26.8
1	A	185	ILE	26.8
1	A	28	SER	26.7
1	B	197	LYS	26.6
1	B	170	SER	26.6
1	C	55	TRP	26.5
1	A	131	ASN	26.5

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Mol	Chain	Res	Type	RSRZ
1	C	187	THR	26.4
1	B	104	GLY	26.4
1	A	106	LEU	26.4
1	B	198	LEU	26.4
1	A	182	ASN	26.3
1	A	63	ALA	26.2
1	B	186	THR	26.2
1	A	127	ASN	26.1
1	B	20	PHE	26.1
1	B	74	LYS	26.0
1	B	65	PHE	26.0
1	B	231	THR	26.0
1	A	108	VAL	25.9
1	B	113	GLY	25.9
1	B	114	ALA	25.8
1	B	133	PRO	25.8
1	D	54	ILE	25.8
1	C	140	ILE	25.8
1	B	64	SER	25.7
1	A	107	GLY	25.7
1	C	64	SER	25.6
1	B	225	PHE	25.6
1	A	96	ILE	25.5
1	B	46	VAL	25.4
1	C	158	GLY	25.4
1	B	123	ASP	25.3
1	C	194	LEU	25.2
1	D	169	SER	25.2
1	C	28	SER	25.2
1	D	158	GLY	25.1
1	D	142	VAL	25.1
1	B	191	VAL	25.1
1	B	75	ASP	25.0
1	A	113	GLY	25.0
1	D	119	GLY	25.0
1	B	68	SER	25.0
1	B	125	TYR	25.0
1	B	5	SER	24.9
1	B	179	THR	24.9
1	C	57	SER	24.8
1	B	127	ASN	24.8
1	B	6	PHE	24.8

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Mol	Chain	Res	Type	RSRZ
1	C	66	LEU	24.8
1	A	205	GLY	24.8
1	A	125	TYR	24.7
1	C	24	VAL	24.7
1	D	155	SER	24.6
1	B	128	SER	24.6
1	D	232	THR	24.6
1	D	135	THR	24.5
1	B	94	THR	24.5
1	C	145	VAL	24.4
1	D	132	ASP	24.4
1	C	56	SER	24.2
1	B	115	GLY	24.1
1	B	107	GLY	24.0
1	B	96	ILE	23.8
1	B	212	LEU	23.8
1	D	123	ASP	23.7
1	D	157	SER	23.6
1	C	61	ASN	23.6
1	A	123	ASP	23.6
1	B	205	GLY	23.5
1	B	120	VAL	23.4
1	D	145	VAL	23.3
1	C	211	SER	23.3
1	C	157	SER	23.3
1	A	130	TYR	23.1
1	D	32	ILE	23.0
1	B	118	VAL	22.7
1	A	216	GLN	22.7
1	C	186	THR	22.7
1	A	148	VAL	22.6
1	C	1	ALA	22.6
1	D	143	ASN	22.6
1	D	134	PRO	22.6
1	B	185	ILE	22.4
1	D	133	PRO	22.4
1	B	138	VAL	22.2
1	B	95	GLN	22.2
1	A	4	VAL	22.2
1	C	72	GLU	22.2
1	A	54	ILE	22.1
1	C	52	VAL	22.1

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Mol	Chain	Res	Type	RSRZ
1	C	26	VAL	22.1
1	D	194	LEU	22.1
1	C	38	ASN	22.0
1	D	95	GLN	21.9
1	A	128	SER	21.9
1	C	78	ASP	21.7
1	C	14	GLY	21.6
1	C	197	LYS	21.6
1	D	1	ALA	21.5
1	A	231	THR	21.5
1	A	126	SER	21.3
1	B	124	THR	21.2
1	C	219	LEU	21.1
1	A	129	GLU	21.0
1	D	198	LEU	20.9
1	B	134	PRO	20.7
1	A	134	PRO	20.6
1	C	159	ALA	20.6
1	C	46	VAL	20.5
1	D	46	VAL	20.3
1	B	126	SER	20.3
1	D	170	SER	20.3
1	A	213	GLY	20.3
1	B	59	THR	20.1
1	B	213	GLY	20.1
1	A	170	SER	20.0
1	C	198	LEU	20.0
1	A	178	VAL	19.8
1	A	114	ALA	19.7
1	D	118	VAL	19.7
1	D	29	ASN	19.7
1	C	156	VAL	19.3
1	C	29	ASN	19.3
1	B	148	VAL	19.1
1	A	57	SER	19.0
1	C	213	GLY	18.4
1	D	38	ASN	18.1
1	C	151	VAL	18.0
1	B	119	GLY	17.9
1	A	177	ALA	17.9
1	B	54	ILE	17.9
1	C	155	SER	17.8

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Mol	Chain	Res	Type	RSRZ
1	D	26	VAL	17.8
1	D	159	ALA	17.8
1	B	149	LYS	17.8
1	D	160	VAL	17.7
1	D	60	GLY	17.7
1	A	217	ILE	17.4
1	B	217	ILE	17.3
1	D	78	ASP	16.6
1	D	112	LYS	16.6
1	D	62	VAL	16.4
1	C	231	THR	16.0
1	C	77	LYS	15.8
1	B	178	VAL	15.6
1	C	160	VAL	15.3
1	B	216	GLN	14.8
1	D	4	VAL	14.6
1	C	112	LYS	14.1
1	C	32	ILE	14.0
1	D	156	VAL	13.6
1	C	232	THR	13.0
1	A	232	THR	12.9
1	D	61	ASN	12.8
1	C	4	VAL	12.1
1	D	77	LYS	12.0
1	B	232	THR	11.9

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.