



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:32 AM 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 X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

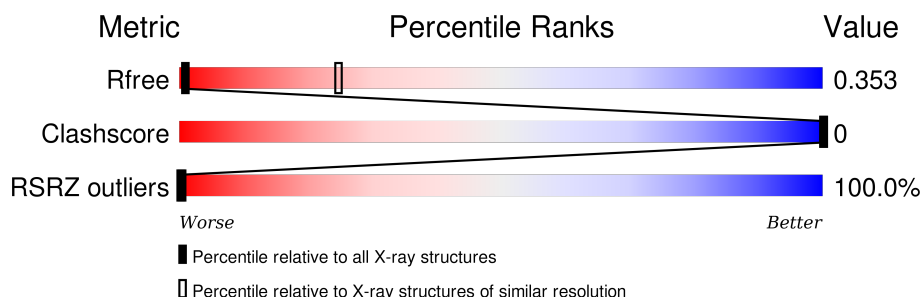
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
RSRZ outliers	91569	1014 (11.50-3.66)

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  $\geq 3$ , 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	236	<p>98% 98% 98% 98% 98% 98%</p>
1	B	236	<p>98% 98% 98% 98% 98% 98%</p>
1	C	236	<p>98% 98% 98% 98% 98% 98%</p>
1	D	236	<p>98% 98% 98% 98% 98% 98%</p>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 928 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.

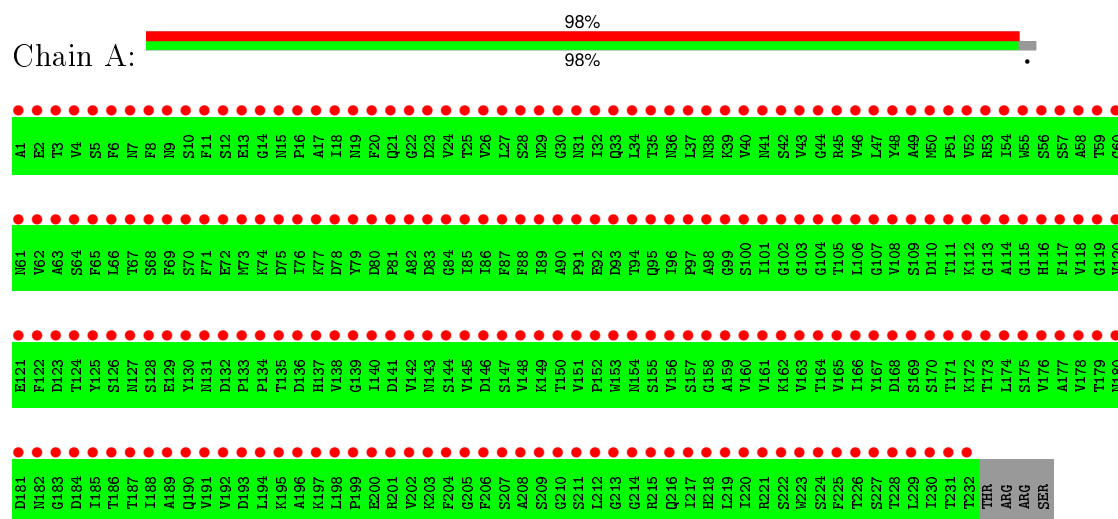
- Molecule 1 is a protein called Galactose-binding lectin.

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

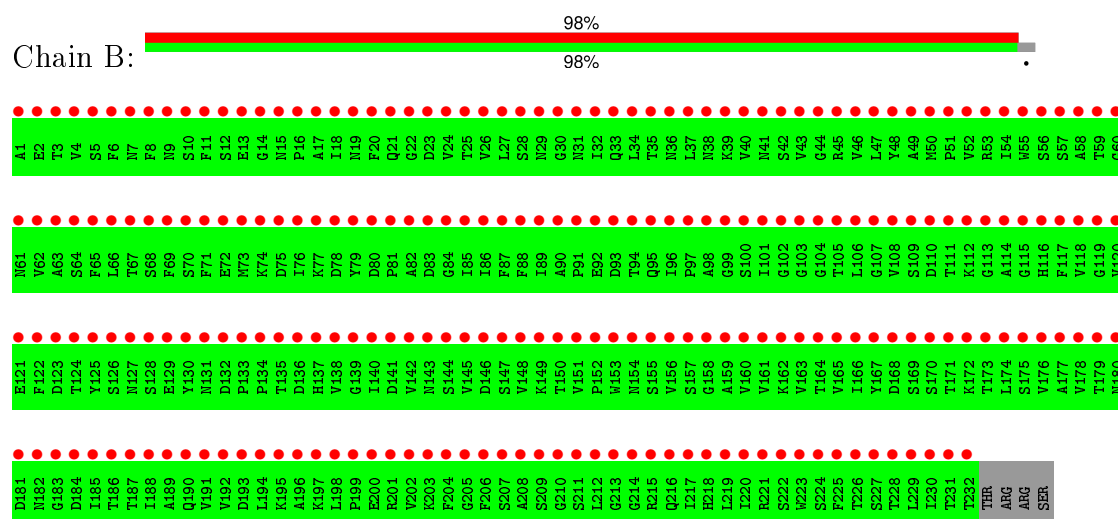
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.42 (at 7.78Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.355 , 0.377 0.369 , 0.353	Depositor DCC
$R_{free}$ test set	104 reflections (4.80%)	DCC
Wilson B-factor (Å <sup>2</sup> )	390.9	Xtriage
Anisotropy	0.950	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	1.00 , 96.0	EDS
Estimated twinning fraction	0.458 for -h,k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

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	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

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 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

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

### 5.3.2 Protein sidechains [i](#)

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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	232/236 (98%)	46.76	232 (100%) 0 0	316, 343, 362, 369	0
1	B	232/236 (98%)	45.87	232 (100%) 0 0	314, 343, 360, 368	0
1	C	232/236 (98%)	44.97	232 (100%) 0 0	321, 354, 371, 375	0
1	D	232/236 (98%)	45.82	232 (100%) 0 0	322, 352, 373, 381	0
All	All	928/944 (98%)	45.86	928 (100%) 0 0	314, 349, 368, 381	0

All (928) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	31	ASN	178.7
1	C	109	SER	170.6
1	B	175	SER	144.0
1	B	30	GLY	127.3
1	C	136	ASP	124.9
1	C	107	GLY	120.2
1	B	189	ALA	119.7
1	A	42	SER	115.3
1	A	71	PHE	114.3
1	D	109	SER	110.1
1	C	105	THR	106.7
1	B	109	SER	106.6
1	C	209	SER	105.6
1	C	208	ALA	103.7
1	C	110	ASP	103.7
1	B	27	LEU	103.4
1	B	42	SER	101.8
1	A	23	ASP	97.9
1	D	152	PRO	97.5
1	D	202	VAL	95.9
1	D	110	ASP	95.8

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Mol	Chain	Res	Type	RSRZ
1	C	115	GLY	95.7
1	C	203	LYS	95.3
1	B	40	VAL	95.2
1	C	201	ARG	94.9
1	C	202	VAL	94.7
1	D	175	SER	93.0
1	B	10	SER	92.2
1	C	175	SER	92.1
1	C	97	PRO	91.7
1	A	33	GLN	91.7
1	D	136	ASP	91.5
1	B	23	ASP	89.2
1	D	201	ARG	88.9
1	A	136	ASP	88.4
1	A	34	LEU	87.9
1	A	155	SER	87.5
1	D	75	ASP	87.3
1	D	203	LYS	87.1
1	D	35	THR	87.0
1	C	224	SER	85.3
1	C	99	GLY	84.8
1	A	26	VAL	84.2
1	C	207	SER	84.1
1	A	41	ASN	83.6
1	A	175	SER	81.6
1	C	106	LEU	81.2
1	A	167	TYR	81.2
1	A	220	ILE	80.9
1	D	207	SER	80.5
1	D	224	SER	80.4
1	D	92	GLU	79.9
1	C	114	ALA	79.6
1	A	203	LYS	79.4
1	B	49	ALA	79.4
1	B	22	GLY	78.4
1	D	105	THR	78.4
1	B	182	ASN	78.1
1	C	7	ASN	77.8
1	A	159	ALA	77.4
1	D	23	ASP	77.3
1	D	99	GLY	76.6
1	D	68	SER	76.0

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Mol	Chain	Res	Type	RSRZ
1	A	92	GLU	75.4
1	C	35	THR	75.2
1	D	222	SER	74.9
1	A	31	ASN	74.8
1	A	72	GLU	74.6
1	D	51	PRO	74.5
1	A	49	ALA	74.5
1	A	13	GLU	74.5
1	B	39	LYS	74.4
1	B	154	ASN	74.2
1	A	165	VAL	73.9
1	B	41	ASN	73.8
1	A	10	SER	73.8
1	B	141	ASP	73.3
1	D	115	GLY	72.3
1	D	42	SER	72.2
1	A	141	ASP	71.4
1	A	202	VAL	71.3
1	D	229	LEU	71.2
1	D	131	ASN	70.4
1	A	93	ASP	70.2
1	D	41	ASN	69.8
1	A	80	ASP	69.8
1	C	147	SER	69.7
1	B	202	VAL	69.3
1	B	2	GLU	69.3
1	D	98	ALA	69.2
1	D	19	ASN	69.2
1	D	204	PHE	69.2
1	C	165	VAL	69.1
1	B	219	LEU	68.9
1	A	183	GLY	68.7
1	A	173	THR	68.6
1	B	203	LYS	68.6
1	A	87	PHE	68.6
1	B	53	ARG	68.4
1	D	44	GLY	68.4
1	D	107	GLY	68.3
1	A	70	SER	68.3
1	B	26	VAL	68.2
1	D	164	THR	68.0
1	A	156	VAL	67.9

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Mol	Chain	Res	Type	RSRZ
1	C	86	ILE	67.9
1	B	57	SER	67.7
1	A	86	ILE	67.6
1	B	152	PRO	67.4
1	B	34	LEU	67.4
1	A	29	ASN	67.1
1	D	165	VAL	67.0
1	A	19	ASN	66.7
1	B	92	GLU	66.6
1	C	128	SER	66.6
1	D	97	PRO	66.5
1	A	207	SER	66.5
1	C	98	ALA	66.3
1	D	69	PHE	66.3
1	C	123	ASP	66.2
1	C	174	LEU	66.1
1	D	221	ARG	65.8
1	D	74	LYS	65.7
1	D	208	ALA	65.6
1	A	174	LEU	65.4
1	B	32	ILE	65.3
1	A	40	VAL	65.2
1	C	22	GLY	65.0
1	B	201	ARG	64.8
1	A	210	GLY	64.7
1	D	67	THR	64.3
1	C	43	VAL	64.2
1	A	30	GLY	64.0
1	D	193	ASP	63.9
1	B	55	TRP	63.8
1	A	154	ASN	63.7
1	A	180	ASN	63.7
1	C	121	GLU	63.7
1	B	153	TRP	63.6
1	B	176	VAL	63.4
1	A	61	ASN	63.3
1	B	99	GLY	63.2
1	D	230	ILE	63.2
1	D	162	LYS	62.9
1	A	160	VAL	62.6
1	C	204	PHE	62.6
1	A	153	TRP	62.4

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Mol	Chain	Res	Type	RSRZ
1	C	83	ASP	62.4
1	D	223	TRP	62.2
1	A	12	SER	62.1
1	A	211	SER	62.1
1	A	68	SER	62.0
1	C	88	PHE	62.0
1	C	6	PHE	61.9
1	B	210	GLY	61.9
1	B	155	SER	61.8
1	A	208	ALA	61.6
1	D	231	THR	61.5
1	B	36	ASN	61.2
1	A	39	LYS	61.0
1	B	181	ASP	61.0
1	A	121	GLU	60.9
1	A	219	LEU	60.8
1	B	9	ASN	60.8
1	D	228	THR	60.8
1	D	39	LYS	60.7
1	C	68	SER	60.7
1	D	215	ARG	60.6
1	C	16	PRO	60.6
1	D	102	GLY	60.5
1	D	163	VAL	60.3
1	D	34	LEU	60.3
1	A	166	ILE	60.2
1	B	3	THR	60.0
1	A	35	THR	59.8
1	A	226	THR	59.8
1	D	153	TRP	59.7
1	B	70	SER	59.7
1	A	164	THR	59.4
1	A	5	SER	59.4
1	A	137	HIS	59.4
1	D	211	SER	59.3
1	B	33	GLN	59.3
1	D	147	SER	59.0
1	D	52	VAL	58.9
1	C	44	GLY	58.7
1	A	163	VAL	58.7
1	B	71	PHE	58.4
1	D	180	ASN	58.4

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Mol	Chain	Res	Type	RSRZ
1	D	176	VAL	58.3
1	A	15	ASN	58.1
1	B	174	LEU	58.1
1	B	52	VAL	58.0
1	C	51	PRO	57.9
1	A	97	PRO	57.9
1	D	154	ASN	57.9
1	C	30	GLY	57.7
1	B	38	ASN	57.7
1	A	21	GLN	57.7
1	A	8	PHE	57.6
1	C	70	SER	57.6
1	C	173	THR	57.4
1	D	137	HIS	57.3
1	A	9	ASN	57.3
1	A	195	LYS	57.2
1	C	144	SER	57.2
1	B	81	PRO	57.2
1	C	100	SER	57.1
1	B	44	GLY	57.1
1	A	206	PHE	57.0
1	C	153	TRP	56.9
1	B	159	ALA	56.9
1	B	29	ASN	56.8
1	C	75	ASP	56.7
1	D	17	ALA	56.5
1	A	150	THR	56.5
1	A	38	ASN	56.4
1	D	33	GLN	56.3
1	D	166	ILE	56.1
1	C	141	ASP	56.1
1	C	89	ILE	56.1
1	D	93	ASP	56.1
1	B	167	TYR	55.9
1	B	97	PRO	55.9
1	D	70	SER	55.8
1	A	214	GLY	55.8
1	A	53	ARG	55.8
1	A	193	ASP	55.8
1	D	81	PRO	55.7
1	B	183	GLY	55.7
1	B	220	ILE	55.7

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Mol	Chain	Res	Type	RSRZ
1	B	209	SER	55.5
1	D	205	GLY	55.5
1	B	80	ASP	55.4
1	A	27	LEU	55.4
1	B	15	ASN	55.2
1	C	81	PRO	55.2
1	C	5	SER	54.9
1	A	78	ASP	54.9
1	C	82	ALA	54.7
1	A	48	TYR	54.7
1	D	45	ARG	54.7
1	B	83	ASP	54.6
1	B	229	LEU	54.5
1	C	85	ILE	54.5
1	A	32	ILE	54.4
1	B	157	SER	54.1
1	A	36	ASN	54.1
1	C	228	THR	53.9
1	B	8	PHE	53.7
1	D	121	GLU	53.7
1	A	222	SER	53.6
1	D	7	ASN	53.6
1	B	130	TYR	53.6
1	D	49	ALA	53.5
1	C	122	PHE	53.5
1	B	208	ALA	53.4
1	B	173	THR	53.3
1	D	10	SER	53.3
1	C	17	ALA	53.3
1	B	72	GLU	53.3
1	B	140	ILE	53.2
1	A	168	ASP	53.2
1	B	156	VAL	53.2
1	D	22	GLY	52.9
1	A	228	THR	52.9
1	D	227	SER	52.8
1	C	69	PHE	52.7
1	A	224	SER	52.7
1	D	113	GLY	52.6
1	C	164	THR	52.6
1	C	223	TRP	52.5
1	B	146	ASP	52.4

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Mol	Chain	Res	Type	RSRZ
1	A	73	MET	52.4
1	D	86	ILE	52.4
1	B	87	PHE	52.3
1	B	221	ARG	52.2
1	B	91	PRO	52.2
1	B	151	VAL	52.2
1	C	176	VAL	52.1
1	D	196	ALA	52.0
1	D	16	PRO	51.9
1	B	105	THR	51.8
1	C	192	VAL	51.6
1	D	104	GLY	51.6
1	A	76	ILE	51.6
1	C	205	GLY	51.5
1	B	12	SER	51.5
1	A	91	PRO	51.4
1	A	7	ASN	51.3
1	D	216	GLN	51.3
1	A	201	ARG	51.2
1	B	14	GLY	51.2
1	D	128	SER	51.2
1	D	30	GLY	51.1
1	B	108	VAL	51.0
1	B	21	GLN	50.8
1	D	80	ASP	50.8
1	C	227	SER	50.7
1	C	49	ALA	50.5
1	A	3	THR	50.4
1	B	28	SER	50.4
1	C	108	VAL	50.4
1	B	222	SER	50.4
1	D	209	SER	50.4
1	A	110	ASP	50.4
1	B	61	ASN	50.3
1	D	87	PHE	50.2
1	D	103	GLY	50.2
1	A	69	PHE	50.2
1	C	10	SER	50.2
1	C	216	GLN	50.1
1	B	190	GLN	50.0
1	C	94	THR	49.8
1	A	147	SER	49.8

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Mol	Chain	Res	Type	RSRZ
1	B	50	MET	49.8
1	C	102	GLY	49.7
1	C	116	HIS	49.7
1	D	192	VAL	49.5
1	B	56	SER	49.4
1	C	222	SER	49.4
1	C	96	ILE	49.4
1	C	193	ASP	49.4
1	D	226	THR	49.4
1	A	184	ASP	49.2
1	A	157	SER	49.2
1	C	167	TYR	49.1
1	A	209	SER	49.1
1	C	180	ASN	49.1
1	B	193	ASP	49.1
1	B	24	VAL	49.1
1	A	109	SER	49.1
1	A	227	SER	49.0
1	C	21	GLN	49.0
1	B	164	THR	49.0
1	A	77	LYS	48.9
1	C	74	LYS	48.9
1	B	206	PHE	48.8
1	A	221	ARG	48.8
1	B	142	VAL	48.7
1	B	25	THR	48.7
1	A	20	PHE	48.7
1	B	110	ASP	48.7
1	C	48	TYR	48.5
1	C	210	GLY	48.5
1	D	83	ASP	48.4
1	B	100	SER	48.3
1	D	100	SER	48.3
1	C	23	ASP	48.3
1	C	200	GLU	48.3
1	D	43	VAL	48.3
1	B	48	TYR	48.3
1	B	98	ALA	48.2
1	A	100	SER	48.2
1	D	124	THR	48.0
1	B	18	ILE	48.0
1	C	172	LYS	47.9

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Mol	Chain	Res	Type	RSRZ
1	A	14	GLY	47.9
1	B	77	LYS	47.9
1	A	89	ILE	47.9
1	C	19	ASN	47.9
1	C	42	SER	47.9
1	A	223	TRP	47.8
1	D	214	GLY	47.8
1	A	218	HIS	47.7
1	B	35	THR	47.6
1	C	137	HIS	47.5
1	A	43	VAL	47.4
1	B	158	GLY	47.4
1	D	150	THR	47.4
1	D	127	ASN	47.3
1	B	163	VAL	47.2
1	B	143	ASN	47.1
1	D	50	MET	47.1
1	A	83	ASP	47.1
1	B	16	PRO	47.0
1	B	86	ILE	47.0
1	A	44	GLY	46.9
1	C	191	VAL	46.9
1	A	230	ILE	46.8
1	B	194	LEU	46.8
1	D	88	PHE	46.7
1	C	220	ILE	46.7
1	C	15	ASN	46.7
1	A	18	ILE	46.6
1	A	176	VAL	46.6
1	C	143	ASN	46.6
1	D	116	HIS	46.5
1	A	146	ASP	46.5
1	A	6	PHE	46.5
1	A	85	ILE	46.4
1	D	82	ALA	46.4
1	C	67	THR	46.3
1	B	93	ASP	46.3
1	A	169	SER	46.3
1	D	24	VAL	46.2
1	C	169	SER	46.2
1	D	183	GLY	46.2
1	C	131	ASN	46.2

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Mol	Chain	Res	Type	RSRZ
1	C	206	PHE	46.0
1	A	24	VAL	46.0
1	D	148	VAL	46.0
1	C	12	SER	45.8
1	C	142	VAL	45.8
1	C	183	GLY	45.8
1	C	170	SER	45.5
1	A	62	VAL	45.4
1	D	190	GLN	45.2
1	B	214	GLY	45.1
1	B	196	ALA	45.0
1	D	210	GLY	45.0
1	C	104	GLY	44.8
1	A	151	VAL	44.8
1	C	58	ALA	44.7
1	D	206	PHE	44.7
1	C	91	PRO	44.7
1	D	12	SER	44.7
1	A	88	PHE	44.5
1	B	218	HIS	44.4
1	D	91	PRO	44.4
1	D	64	SER	44.3
1	A	17	ALA	44.2
1	C	226	THR	44.2
1	C	120	VAL	44.2
1	A	50	MET	44.1
1	B	168	ASP	44.1
1	C	92	GLU	44.1
1	B	200	GLU	44.0
1	B	207	SER	44.0
1	D	181	ASP	44.0
1	C	84	GLY	44.0
1	B	79	TYR	44.0
1	A	117	PHE	44.0
1	D	173	THR	44.0
1	C	179	THR	43.8
1	D	15	ASN	43.7
1	B	13	GLU	43.6
1	A	75	ASP	43.6
1	C	196	ALA	43.6
1	D	14	GLY	43.6
1	D	48	TYR	43.5

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Mol	Chain	Res	Type	RSRZ
1	C	125	TYR	43.5
1	A	143	ASN	43.5
1	A	158	GLY	43.5
1	C	41	ASN	43.5
1	D	89	ILE	43.4
1	B	169	SER	43.4
1	D	182	ASN	43.4
1	C	184	ASP	43.4
1	D	9	ASN	43.4
1	C	139	GLY	43.4
1	A	122	PHE	43.2
1	B	11	PHE	43.2
1	C	189	ALA	43.2
1	C	214	GLY	43.1
1	D	90	ALA	43.1
1	B	85	ILE	43.1
1	B	103	GLY	42.9
1	D	140	ILE	42.9
1	D	37	LEU	42.9
1	A	111	THR	42.9
1	B	228	THR	42.8
1	D	187	THR	42.8
1	B	227	SER	42.8
1	C	90	ALA	42.7
1	C	124	THR	42.7
1	A	172	LYS	42.5
1	B	160	VAL	42.4
1	C	129	GLU	42.4
1	D	76	ILE	42.4
1	B	62	VAL	42.4
1	A	189	ALA	42.4
1	D	25	THR	42.3
1	B	144	SER	42.3
1	D	171	THR	42.3
1	A	196	ALA	42.3
1	C	47	LEU	42.2
1	C	190	GLN	42.2
1	C	166	ILE	42.1
1	A	229	LEU	42.0
1	C	9	ASN	42.0
1	C	127	ASN	41.9
1	B	147	SER	41.8

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Mol	Chain	Res	Type	RSRZ
1	C	36	ASN	41.8
1	D	28	SER	41.8
1	C	163	VAL	41.8
1	B	60	GLY	41.8
1	B	223	TRP	41.7
1	B	7	ASN	41.7
1	A	99	GLY	41.7
1	D	101	ILE	41.6
1	D	106	LEU	41.6
1	D	47	LEU	41.6
1	B	131	ASN	41.5
1	D	177	ALA	41.5
1	D	36	ASN	41.4
1	C	87	PHE	41.4
1	D	96	ILE	41.3
1	A	16	PRO	41.2
1	B	19	ASN	41.2
1	B	172	LYS	41.2
1	B	69	PHE	41.1
1	D	200	GLU	41.1
1	D	66	LEU	41.1
1	C	25	THR	41.1
1	C	168	ASP	41.1
1	A	215	ARG	41.0
1	C	111	THR	41.0
1	C	221	ARG	41.0
1	A	152	PRO	40.9
1	C	59	THR	40.8
1	B	73	MET	40.8
1	A	67	THR	40.7
1	B	102	GLY	40.6
1	D	13	GLU	40.6
1	A	84	GLY	40.5
1	A	103	GLY	40.5
1	B	136	ASP	40.5
1	B	204	PHE	40.4
1	C	215	ARG	40.3
1	B	43	VAL	40.3
1	D	58	ALA	40.3
1	D	27	LEU	40.2
1	D	31	ASN	40.2
1	B	211	SER	40.1

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Mol	Chain	Res	Type	RSRZ
1	B	226	THR	40.1
1	C	71	PHE	40.1
1	A	90	ALA	40.1
1	B	51	PRO	40.1
1	D	169	SER	40.1
1	A	132	ASP	40.0
1	C	113	GLY	39.9
1	B	184	ASP	39.9
1	D	21	GLN	39.9
1	D	144	SER	39.9
1	B	171	THR	39.8
1	B	121	GLU	39.8
1	D	178	VAL	39.8
1	A	133	PRO	39.6
1	B	111	THR	39.6
1	B	224	SER	39.6
1	D	11	PHE	39.5
1	A	98	ALA	39.5
1	C	126	SER	39.5
1	C	171	THR	39.5
1	A	105	THR	39.3
1	D	172	LYS	39.2
1	B	180	ASN	39.2
1	B	192	VAL	39.2
1	A	55	TRP	39.1
1	A	52	VAL	39.1
1	C	45	ARG	39.1
1	B	165	VAL	39.0
1	D	65	PHE	39.0
1	A	135	THR	39.0
1	D	149	LYS	39.0
1	A	142	VAL	38.9
1	C	117	PHE	38.9
1	D	191	VAL	38.8
1	A	140	ILE	38.7
1	B	101	ILE	38.7
1	A	120	VAL	38.7
1	A	197	LYS	38.7
1	B	116	HIS	38.7
1	D	220	ILE	38.6
1	D	174	LEU	38.5
1	D	189	ALA	38.5

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Mol	Chain	Res	Type	RSRZ
1	D	212	LEU	38.3
1	B	78	ASP	38.2
1	A	139	GLY	38.2
1	D	72	GLU	38.2
1	D	168	ASP	38.2
1	C	39	LYS	38.1
1	D	161	VAL	38.0
1	C	53	ARG	37.9
1	D	225	PHE	37.9
1	D	94	THR	37.8
1	C	101	ILE	37.7
1	D	56	SER	37.7
1	A	82	ALA	37.6
1	A	225	PHE	37.6
1	B	215	ARG	37.5
1	D	218	HIS	37.5
1	B	37	LEU	37.5
1	A	188	ILE	37.4
1	A	74	LYS	37.4
1	C	63	ALA	37.4
1	C	154	ASN	37.4
1	B	67	THR	37.4
1	D	79	TYR	37.3
1	D	5	SER	37.2
1	A	60	GLY	37.1
1	B	76	ILE	37.1
1	A	161	VAL	37.1
1	C	80	ASP	37.1
1	A	56	SER	37.1
1	B	84	GLY	37.0
1	D	57	SER	37.0
1	D	3	THR	36.9
1	C	119	GLY	36.8
1	B	88	PHE	36.8
1	A	181	ASP	36.6
1	D	108	VAL	36.6
1	A	45	ARG	36.5
1	A	145	VAL	36.4
1	A	118	VAL	36.4
1	B	47	LEU	36.4
1	C	18	ILE	36.3
1	C	150	THR	36.3

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Mol	Chain	Res	Type	RSRZ
1	A	64	SER	36.2
1	D	126	SER	36.0
1	C	93	ASP	36.0
1	A	28	SER	36.0
1	C	230	ILE	35.9
1	D	18	ILE	35.9
1	C	162	LYS	35.8
1	A	190	GLN	35.7
1	A	144	SER	35.7
1	B	161	VAL	35.7
1	C	225	PHE	35.7
1	D	122	PHE	35.5
1	D	186	THR	35.5
1	C	229	LEU	35.4
1	D	170	SER	35.4
1	D	84	GLY	35.4
1	B	187	THR	35.4
1	A	22	GLY	35.3
1	A	192	VAL	35.3
1	B	4	VAL	35.2
1	C	118	VAL	35.2
1	C	65	PHE	35.1
1	B	145	VAL	35.1
1	C	152	PRO	35.0
1	C	37	LEU	35.0
1	C	34	LEU	35.0
1	B	64	SER	34.9
1	B	170	SER	34.9
1	C	40	VAL	34.9
1	C	146	ASP	34.8
1	A	119	GLY	34.7
1	B	89	ILE	34.7
1	C	181	ASP	34.7
1	B	17	ALA	34.7
1	D	8	PHE	34.6
1	D	53	ARG	34.6
1	D	179	THR	34.5
1	C	76	ILE	34.5
1	B	5	SER	34.5
1	D	85	ILE	34.5
1	C	64	SER	34.5
1	C	148	VAL	34.4

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Mol	Chain	Res	Type	RSRZ
1	D	141	ASP	34.4
1	B	1	ALA	34.4
1	A	2	GLU	34.4
1	D	6	PHE	34.4
1	A	187	THR	34.2
1	C	28	SER	34.2
1	C	103	GLY	34.2
1	A	191	VAL	34.2
1	D	55	TRP	34.2
1	D	59	THR	34.1
1	C	161	VAL	34.0
1	A	51	PRO	34.0
1	C	57	SER	33.9
1	D	146	ASP	33.9
1	A	204	PHE	33.8
1	D	114	ALA	33.8
1	D	139	GLY	33.8
1	C	31	ASN	33.8
1	A	81	PRO	33.6
1	B	162	LYS	33.6
1	B	128	SER	33.5
1	D	111	THR	33.5
1	A	102	GLY	33.4
1	A	131	ASN	33.4
1	C	62	VAL	33.4
1	A	79	TYR	33.3
1	D	138	VAL	33.3
1	A	104	GLY	33.2
1	B	68	SER	33.2
1	D	125	TYR	33.1
1	A	124	THR	33.1
1	A	101	ILE	33.1
1	B	82	ALA	33.1
1	B	195	LYS	33.1
1	D	184	ASP	33.0
1	C	11	PHE	33.0
1	A	179	THR	33.0
1	A	25	THR	33.0
1	B	132	ASP	32.9
1	D	155	SER	32.9
1	A	138	VAL	32.9
1	D	40	VAL	32.7

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Mol	Chain	Res	Type	RSRZ
1	C	182	ASN	32.6
1	A	212	LEU	32.5
1	C	177	ALA	32.5
1	A	127	ASN	32.5
1	A	58	ALA	32.5
1	C	56	SER	32.4
1	A	37	LEU	32.3
1	A	46	VAL	32.3
1	C	211	SER	32.3
1	D	20	PHE	32.2
1	D	73	MET	32.2
1	D	167	TYR	32.2
1	D	185	ILE	32.2
1	A	94	THR	32.2
1	B	66	LEU	32.1
1	C	50	MET	32.1
1	A	194	LEU	32.1
1	B	139	GLY	32.1
1	C	149	LYS	32.1
1	C	188	ILE	31.9
1	D	63	ALA	31.8
1	C	157	SER	31.8
1	B	135	THR	31.7
1	C	132	ASP	31.7
1	C	8	PHE	31.6
1	A	182	ASN	31.5
1	D	157	SER	31.5
1	B	188	ILE	31.4
1	D	195	LYS	31.4
1	D	217	ILE	31.3
1	B	117	PHE	31.1
1	C	3	THR	31.1
1	A	162	LYS	31.0
1	B	177	ALA	30.9
1	D	130	TYR	30.9
1	A	171	THR	30.8
1	C	13	GLU	30.6
1	B	127	ASN	30.6
1	D	117	PHE	30.6
1	B	137	HIS	30.5
1	C	133	PRO	30.5
1	C	135	THR	30.4

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Mol	Chain	Res	Type	RSRZ
1	D	120	VAL	30.4
1	B	129	GLU	30.3
1	A	59	THR	30.2
1	D	129	GLU	30.1
1	C	195	LYS	30.1
1	C	138	VAL	30.1
1	D	219	LEU	30.1
1	D	151	VAL	30.0
1	B	112	LYS	30.0
1	D	213	GLY	29.9
1	B	122	PHE	29.9
1	A	65	PHE	29.8
1	C	20	PHE	29.8
1	C	178	VAL	29.8
1	A	186	THR	29.7
1	D	2	GLU	29.7
1	C	218	HIS	29.7
1	B	166	ILE	29.7
1	A	128	SER	29.6
1	A	200	GLU	29.5
1	B	75	ASP	29.4
1	B	123	ASP	29.3
1	B	90	ALA	29.2
1	B	106	LEU	29.2
1	A	47	LEU	29.0
1	D	71	PHE	29.0
1	A	115	GLY	29.0
1	A	11	PHE	29.0
1	B	63	ALA	28.9
1	B	150	THR	28.9
1	C	130	TYR	28.9
1	B	104	GLY	28.8
1	A	149	LYS	28.7
1	D	132	ASP	28.5
1	A	126	SER	28.5
1	B	230	ILE	28.5
1	A	1	ALA	28.4
1	A	116	HIS	28.3
1	A	95	GLN	28.3
1	B	113	GLY	28.2
1	C	158	GLY	28.1
1	A	198	LEU	28.0

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Mol	Chain	Res	Type	RSRZ
1	D	143	ASN	28.0
1	C	60	GLY	27.9
1	C	199	PRO	27.9
1	C	61	ASN	27.9
1	B	45	ARG	27.8
1	C	217	ILE	27.7
1	A	107	GLY	27.7
1	B	186	THR	27.7
1	C	212	LEU	27.6
1	B	58	ALA	27.6
1	D	123	ASP	27.6
1	C	54	ILE	27.5
1	C	134	PRO	27.5
1	C	187	THR	27.5
1	B	231	THR	27.4
1	C	185	ILE	27.4
1	B	179	THR	27.3
1	D	142	VAL	27.1
1	B	6	PHE	27.1
1	A	123	ASP	27.1
1	D	119	GLY	26.9
1	B	65	PHE	26.9
1	A	108	VAL	26.9
1	B	115	GLY	26.9
1	B	46	VAL	26.9
1	B	126	SER	26.9
1	C	33	GLN	26.9
1	D	188	ILE	26.8
1	B	225	PHE	26.8
1	A	113	GLY	26.8
1	C	2	GLU	26.8
1	C	55	TRP	26.7
1	D	158	GLY	26.7
1	B	20	PHE	26.6
1	C	24	VAL	26.6
1	B	199	PRO	26.6
1	C	95	GLN	26.4
1	A	205	GLY	26.3
1	D	135	THR	26.2
1	B	191	VAL	26.1
1	C	38	ASN	26.0
1	B	114	ALA	26.0

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Mol	Chain	Res	Type	RSRZ
1	D	232	THR	26.0
1	A	170	SER	25.9
1	C	27	LEU	25.8
1	B	94	THR	25.8
1	B	205	GLY	25.7
1	B	120	VAL	25.6
1	A	66	LEU	25.5
1	B	107	GLY	25.5
1	D	199	PRO	25.4
1	A	57	SER	25.3
1	A	199	PRO	25.2
1	B	133	PRO	25.2
1	A	63	ALA	25.2
1	C	145	VAL	25.2
1	D	145	VAL	25.1
1	A	112	LYS	24.9
1	B	197	LYS	24.8
1	C	29	ASN	24.8
1	D	197	LYS	24.7
1	A	148	VAL	24.5
1	C	79	TYR	24.2
1	A	185	ILE	24.1
1	B	118	VAL	24.0
1	C	155	SER	23.9
1	B	74	LYS	23.9
1	C	78	ASP	23.7
1	C	140	ILE	23.7
1	B	138	VAL	23.5
1	D	38	ASN	23.4
1	C	186	THR	23.3
1	D	54	ILE	23.3
1	C	14	GLY	23.3
1	D	29	ASN	23.3
1	C	52	VAL	23.1
1	A	96	ILE	23.0
1	B	198	LEU	22.7
1	C	26	VAL	22.7
1	C	73	MET	22.7
1	A	4	VAL	22.6
1	B	124	THR	22.5
1	D	133	PRO	22.4
1	A	106	LEU	22.4

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Mol	Chain	Res	Type	RSRZ
1	A	231	THR	22.3
1	D	134	PRO	22.2
1	A	213	GLY	21.9
1	C	1	ALA	21.9
1	B	213	GLY	21.8
1	C	46	VAL	21.6
1	C	194	LEU	21.6
1	B	96	ILE	21.6
1	A	216	GLN	21.4
1	B	59	THR	21.3
1	B	125	TYR	21.2
1	B	95	GLN	21.1
1	D	46	VAL	21.1
1	C	66	LEU	21.0
1	A	125	TYR	20.9
1	D	32	ILE	20.9
1	C	72	GLU	20.8
1	D	1	ALA	20.8
1	D	95	GLN	20.8
1	B	185	ILE	20.7
1	D	118	VAL	20.7
1	B	212	LEU	20.5
1	A	130	TYR	20.5
1	C	159	ALA	20.4
1	B	134	PRO	20.1
1	D	60	GLY	20.0
1	A	54	ILE	20.0
1	A	129	GLU	20.0
1	C	213	GLY	19.9
1	C	156	VAL	19.9
1	A	134	PRO	19.9
1	D	78	ASP	19.9
1	B	148	VAL	19.8
1	B	119	GLY	19.6
1	A	178	VAL	19.5
1	C	197	LYS	19.5
1	D	26	VAL	19.5
1	C	151	VAL	19.2
1	A	114	ALA	18.9
1	D	194	LEU	18.8
1	C	219	LEU	18.7
1	D	160	VAL	18.3

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Mol	Chain	Res	Type	RSRZ
1	D	62	VAL	17.5
1	D	198	LEU	17.3
1	A	177	ALA	17.1
1	C	231	THR	17.0
1	D	159	ALA	17.0
1	C	198	LEU	16.7
1	B	178	VAL	16.7
1	C	160	VAL	16.5
1	D	61	ASN	16.2
1	B	54	ILE	16.2
1	A	217	ILE	16.0
1	B	149	LYS	15.8
1	B	217	ILE	15.4
1	D	112	LYS	15.0
1	D	4	VAL	14.9
1	C	77	LYS	14.5
1	D	156	VAL	14.3
1	B	216	GLN	14.0
1	C	232	THR	13.6
1	A	232	THR	13.3
1	C	112	LYS	13.0
1	C	4	VAL	12.7
1	C	32	ILE	12.5
1	B	232	THR	12.3
1	D	77	LYS	11.3

## 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 [i](#)

There are no such residues in this entry.