



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:21 AM GMT

PDB ID : 3MZK
Title : Sec13/Sec16 complex, S.cerevisiae
Authors : Whittle, J.R.; Schwartz, T.U.
Deposited on : 2010-05-12
Resolution : 2.69 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>

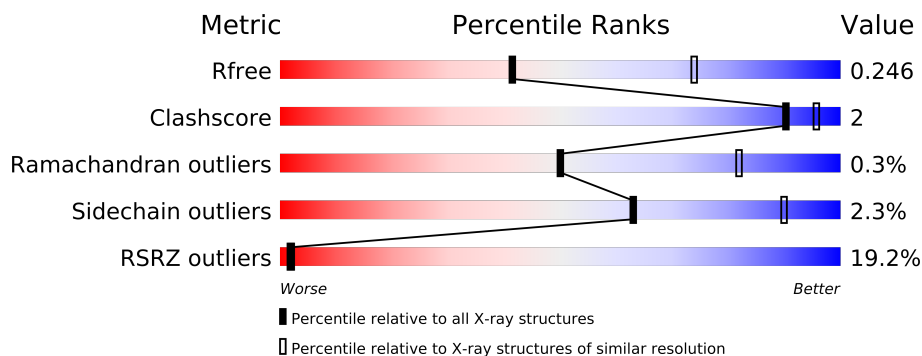
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.69 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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	297	
1	D	297	
2	B	441	
2	C	441	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10662 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 Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2329	1481	400	444	4			
1	D	297	Total	C	N	O	S	0	0	0
			2322	1477	398	443	4			

- Molecule 2 is a protein called Protein transport protein SEC16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	385	Total	C	N	O	S	0	0	0
			2932	1904	472	544	12			
2	C	381	Total	C	N	O	S	0	0	0
			2904	1890	467	536	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	980	GLY	-	EXPRESSION TAG	UNP P48415
B	981	PRO	-	EXPRESSION TAG	UNP P48415
B	982	GLY	-	EXPRESSION TAG	UNP P48415
B	983	SER	-	EXPRESSION TAG	UNP P48415
C	980	GLY	-	EXPRESSION TAG	UNP P48415
C	981	PRO	-	EXPRESSION TAG	UNP P48415
C	982	GLY	-	EXPRESSION TAG	UNP P48415
C	983	SER	-	EXPRESSION TAG	UNP P48415

- Molecule 3 is water.

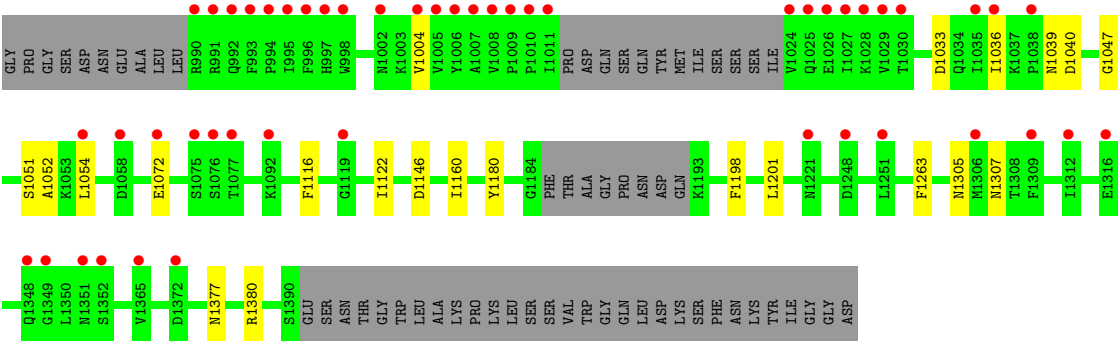
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	116	Total	O	0	0
			116	116		
3	B	48	Total	O	0	0
			48	48		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	10	Total	O	0	0
			10	10		
3	D	1	Total	O	0	0
			1	1		

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.73Å 139.01Å 205.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.71 – 2.69 30.71 – 2.69	Depositor EDS
% Data completeness (in resolution range)	92.3 (30.71-2.69) 98.2 (30.71-2.69)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.198 , 0.243 0.200 , 0.246	Depositor DCC
R_{free} test set	2289 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 57.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 45258 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10662	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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	$\# Z > 5$
1	A	0.34	0/2392	0.53	0/3263
1	D	0.31	0/2385	0.51	0/3255
2	B	0.29	0/2999	0.42	0/4094
2	C	0.24	0/2971	0.41	0/4057
All	All	0.30	0/10747	0.47	0/14669

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	2329	0	0	5	0
1	D	2322	0	0	9	0
2	B	2932	0	3	5	0
2	C	2904	0	0	11	0
3	A	116	0	0	2	0
3	B	48	0	0	2	0
3	C	10	0	0	0	0
3	D	1	0	0	0	0
All	All	10662	0	3	22	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 2.

All (22) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:1380:ARG:CZ	1:D:156:ALA:O	2.36	0.74
2:B:1132:CYS:SG	2:C:1116:PHE:CZ	2.97	0.57
2:C:1377:ASN:OD1	1:D:158:ILE:N	2.39	0.56
2:C:1305:ASN:N	1:D:285:LEU:O	2.40	0.55
1:A:52:HIS:CD2	1:A:74:SER:CB	2.93	0.51
1:D:52:HIS:CD2	1:D:74:SER:CB	2.94	0.51
2:C:1039:ASN:O	2:C:1039:ASN:OD1	2.30	0.50
2:C:1307:ASN:CB	1:D:283:GLU:OE1	2.60	0.49
2:C:1380:ARG:NH1	1:D:156:ALA:O	2.47	0.48
1:A:68:THR:N	3:A:340:HOH:O	2.45	0.47
2:B:991:ARG:NE	3:B:291:HOH:O	2.47	0.47
2:C:1033:ASP:CA	2:C:1036:ILE:O	2.63	0.47
1:A:7:ALA:N	3:A:351:HOH:O	2.49	0.46
1:D:98:HIS:CE1	1:D:126:SER:OG	2.69	0.45
1:D:296:HIS:O	1:D:297:GLN:C	2.57	0.42
1:A:98:HIS:CE1	1:A:126:SER:OG	2.72	0.42
2:C:1305:ASN:ND2	1:D:283:GLU:CB	2.83	0.41
2:C:1052:ALA:C	2:C:1054:LEU:N	2.72	0.41
2:B:1127:ARG:NH2	2:C:1180:TYR:O	2.54	0.41
2:B:1337:GLN:NE2	3:B:34:HOH:O	2.53	0.41
1:A:296:HIS:O	1:A:297:GLN:C	2.58	0.41
2:B:1052:ALA:C	2:B:1054:LEU:N	2.75	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	295/297 (99%)	278 (94%)	16 (5%)	1 (0%)	50 82
1	D	295/297 (99%)	284 (96%)	10 (3%)	1 (0%)	50 82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	379/441 (86%)	360 (95%)	18 (5%)	1 (0%)	50	82
2	C	375/441 (85%)	347 (92%)	27 (7%)	1 (0%)	50	82
All	All	1344/1476 (91%)	1269 (94%)	71 (5%)	4 (0%)	50	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1047	GLY
2	C	1047	GLY
1	D	202	GLY
1	A	202	GLY

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	250/252 (99%)	246 (98%)	4 (2%)	75	94
1	D	248/252 (98%)	246 (99%)	2 (1%)	89	98
2	B	306/395 (78%)	297 (97%)	9 (3%)	55	85
2	C	302/395 (76%)	292 (97%)	10 (3%)	50	81
All	All	1106/1294 (86%)	1081 (98%)	25 (2%)	63	90

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	SER
1	A	197	GLU
1	A	198	SER
1	A	216	VAL
2	B	1004	VAL
2	B	1051	SER
2	B	1054	LEU
2	B	1072	GLU
2	B	1074	GLU
2	B	1146	ASP

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Mol	Chain	Res	Type
2	B	1160	ILE
2	B	1198	PHE
2	B	1201	LEU
2	C	1004	VAL
2	C	1040	ASP
2	C	1051	SER
2	C	1072	GLU
2	C	1122	ILE
2	C	1146	ASP
2	C	1160	ILE
2	C	1198	PHE
2	C	1201	LEU
2	C	1263	PHE
1	D	197	GLU
1	D	198	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	297/297 (100%)	-0.46	1 (0%) 91 95	20, 39, 90, 133	0
1	D	297/297 (100%)	4.00	207 (69%) 0 0	122, 243, 326, 392	0
2	B	385/441 (87%)	-0.24	4 (1%) 79 83	33, 72, 123, 174	0
2	C	381/441 (86%)	0.59	49 (12%) 4 4	49, 99, 228, 287	0
All	All	1360/1476 (92%)	0.87	261 (19%) 2 2	20, 84, 276, 392	0

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	68	THR	20.6
1	D	67	GLY	16.5
1	D	114	PRO	13.6
1	D	272	SER	13.2
1	D	197	GLU	12.6
1	D	189	SER	12.3
2	C	1010	PRO	12.1
1	D	167	THR	11.7
1	D	87	GLY	11.3
1	D	253	PHE	11.0
1	D	3	VAL	10.6
1	D	181	LEU	10.6
1	D	9	ASN	10.6
2	C	1026	GLU	10.4
1	D	187	TYR	10.4
2	C	1011	ILE	10.3
1	D	6	ASN	10.1
2	C	1009	PRO	10.1
1	D	258	TRP	9.9
2	C	1006	TYR	9.7
1	D	65	LYS	9.7

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Mol	Chain	Res	Type	RSRZ
1	D	7	ALA	9.5
1	D	151	ALA	9.2
1	D	120	SER	9.1
1	D	259	ARG	9.0
2	C	1027	ILE	9.0
1	D	225	VAL	9.0
1	D	49	LEU	8.8
1	D	252	LYS	8.7
1	D	297	GLN	8.6
2	C	1008	VAL	8.5
1	D	104	SER	8.5
1	D	240	GLN	8.4
2	C	1007	ALA	8.2
1	D	56	VAL	8.2
1	D	194	TYR	8.1
1	D	82	TRP	8.0
1	D	251	GLU	7.9
1	D	250	GLU	7.9
1	D	36	PHE	7.8
1	D	13	HIS	7.8
1	D	5	ALA	7.7
1	D	209	ASP	7.6
1	D	23	ARG	7.5
1	D	55	PRO	7.5
1	D	139	ILE	7.4
1	D	296	HIS	7.4
1	D	14	ASP	7.4
1	D	11	LEU	7.3
1	D	89	TRP	7.3
1	D	239	GLU	7.3
1	D	193	THR	7.3
1	D	173	PHE	7.2
1	D	203	HIS	7.2
2	C	996	PHE	7.1
1	D	153	TRP	7.1
1	D	95	HIS	7.1
2	C	991	ARG	6.9
1	D	10	GLU	6.8
1	D	44	LYS	6.7
1	D	160	GLU	6.7
1	D	277	LYS	6.6
1	D	25	ALA	6.6

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Mol	Chain	Res	Type	RSRZ
2	C	1028	LYS	6.6
1	D	261	SER	6.6
1	D	45	LEU	6.5
1	D	271	LEU	6.4
1	D	128	VAL	6.4
2	C	1025	GLN	6.4
1	D	58	ARG	6.3
1	D	234	TRP	6.2
1	D	192	GLN	6.2
1	D	4	ILE	6.2
1	D	1	MET	6.1
1	D	106	GLN	6.0
1	D	8	HIS	6.0
2	C	995	ILE	5.9
1	D	208	ARG	5.9
1	D	57	TRP	5.7
1	D	24	LEU	5.7
1	D	21	GLY	5.7
1	D	143	ALA	5.7
2	C	993	PHE	5.7
1	D	107	TRP	5.6
1	D	119	ALA	5.6
1	D	211	ALA	5.6
1	D	185	TRP	5.6
1	D	130	PHE	5.6
1	D	12	ILE	5.5
1	D	269	LEU	5.5
1	D	281	TRP	5.5
1	D	37	GLU	5.5
2	C	992	GLN	5.5
1	D	255	ASP	5.5
1	D	117	LEU	5.4
2	C	1024	VAL	5.4
1	D	176	GLY	5.3
1	D	20	TYR	5.3
1	D	257	LEU	5.3
2	C	1002	ASN	5.3
1	D	64	PRO	5.2
1	D	247	LEU	5.2
1	D	212	TRP	5.1
1	D	16	VAL	5.1
2	C	990	ARG	5.1

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Mol	Chain	Res	Type	RSRZ
1	D	73	CYS	5.0
1	D	70	LEU	5.0
1	D	26	THR	5.0
1	D	88	ARG	4.9
1	D	29	SER	4.9
1	D	158	ILE	4.9
1	D	248	LEU	4.8
1	D	60	ASP	4.8
1	D	190	ASP	4.7
1	D	126	SER	4.7
1	D	105	VAL	4.7
1	D	243	TRP	4.7
1	D	142	ASP	4.7
1	D	260	ALA	4.6
2	C	1004	VAL	4.6
1	D	17	LEU	4.6
1	D	133	ASN	4.6
1	D	207	VAL	4.6
1	D	295	VAL	4.5
1	D	224	SER	4.4
2	C	994	PRO	4.3
1	D	141	ILE	4.3
1	D	171	ARG	4.2
1	D	186	LYS	4.2
1	D	206	TRP	4.2
1	D	118	VAL	4.2
1	D	144	HIS	4.2
1	D	15	ALA	4.1
1	D	183	LYS	4.1
1	D	256	VAL	4.1
2	C	997	HIS	4.1
1	D	152	SER	4.1
1	D	169	GLU	4.1
1	D	244	LYS	4.0
1	D	50	THR	4.0
2	C	1092	LYS	4.0
1	D	51	GLY	4.0
1	D	195	VAL	4.0
2	C	1035	ILE	4.0
1	D	27	CYS	4.0
1	D	270	ALA	3.9
2	C	998	TRP	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	59	VAL	3.8
1	D	19	TYR	3.8
2	C	1221	ASN	3.8
1	D	230	THR	3.8
2	C	1030	THR	3.8
1	D	262	TRP	3.8
1	D	78	LYS	3.7
1	D	157	THR	3.7
1	D	71	ALA	3.7
1	D	148	VAL	3.7
1	D	113	GLY	3.6
1	D	226	SER	3.6
1	D	33	ILE	3.6
1	D	61	TRP	3.6
1	D	115	LEU	3.5
1	D	48	THR	3.5
1	D	140	ILE	3.5
1	D	34	LYS	3.5
1	D	174	VAL	3.5
1	D	75	TYR	3.5
2	C	1077	THR	3.5
1	D	63	HIS	3.4
1	D	69	ILE	3.4
1	D	149	ASN	3.4
1	D	92	ILE	3.4
1	D	145	ALA	3.4
1	D	184	ILE	3.4
1	D	41	GLU	3.4
1	D	131	LYS	3.4
2	B	1219	THR	3.3
1	D	32	THR	3.3
1	D	99	SER	3.3
1	D	38	VAL	3.3
1	D	159	GLU	3.3
1	D	90	SER	3.3
1	D	175	THR	3.2
2	C	1076	SER	3.2
1	D	179	ASP	3.2
1	D	86	ASN	3.2
1	D	172	LYS	3.2
1	D	254	PRO	3.2
1	D	154	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	210	VAL	3.2
2	C	1054	LEU	3.1
1	D	137	SER	3.1
1	D	287	GLY	3.1
1	D	217	LEU	3.1
1	D	134	GLY	3.1
1	D	216	VAL	3.1
2	C	1251	LEU	3.1
1	D	98	HIS	3.1
1	D	108	ALA	3.0
2	C	1072	GLU	3.0
1	D	249	LYS	3.0
2	C	1349	GLY	3.0
1	D	290	GLU	3.0
1	D	43	HIS	3.0
1	D	47	ASP	2.9
1	D	127	VAL	2.9
2	C	1351	ASN	2.9
1	D	155	PRO	2.9
1	D	227	GLN	2.9
2	B	1246	ASN	2.8
2	C	1075	SER	2.8
1	D	221	TYR	2.8
1	D	218	LEU	2.8
2	C	1309	PHE	2.8
1	D	62	ALA	2.8
1	D	180	ASN	2.7
1	D	268	VAL	2.7
1	D	116	LEU	2.7
1	D	111	GLU	2.7
1	D	205	ASP	2.7
1	D	223	ALA	2.7
1	D	232	ILE	2.7
1	D	84	GLU	2.6
1	D	42	THR	2.6
2	C	1029	VAL	2.6
1	D	222	LEU	2.6
2	C	1312	ILE	2.5
1	D	103	ASN	2.5
1	D	81	ILE	2.5
1	D	278	VAL	2.5
2	B	1010	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	168	LYS	2.4
1	D	238	ASN	2.4
2	C	1038	PRO	2.4
1	D	22	LYS	2.4
1	D	72	SER	2.4
2	C	1036	ILE	2.4
2	C	1365	VAL	2.4
1	A	88	ARG	2.4
2	C	1005	VAL	2.3
1	D	245	LYS	2.3
1	D	242	PRO	2.3
2	C	1248	ASP	2.3
1	D	292	ALA	2.3
1	D	94	VAL	2.2
2	B	1247	GLU	2.2
1	D	150	SER	2.2
1	D	215	THR	2.2
1	D	246	THR	2.1
1	D	273	GLY	2.1
1	D	200	LEU	2.1
2	C	1352	SER	2.1
2	C	1058	ASP	2.1
2	C	1372	ASP	2.1
1	D	132	GLU	2.1
1	D	135	THR	2.1
2	C	1316	GLU	2.1
2	C	1119	GLY	2.1
2	C	1348	GLN	2.0
2	C	1306	MET	2.0
1	D	97	VAL	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 ⓘ

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.