Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:44 AM GMT

PDB ID	:	3PSF
Title	:	Crystal Structure of the Spt6 core domain from Saccharomyces cerevisiae, Form Spt6(236-1259)
Authors	:	Close, D.; Hill, C.P.
Deposited on	:	2010-12-01
Resolution	:	2.59 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

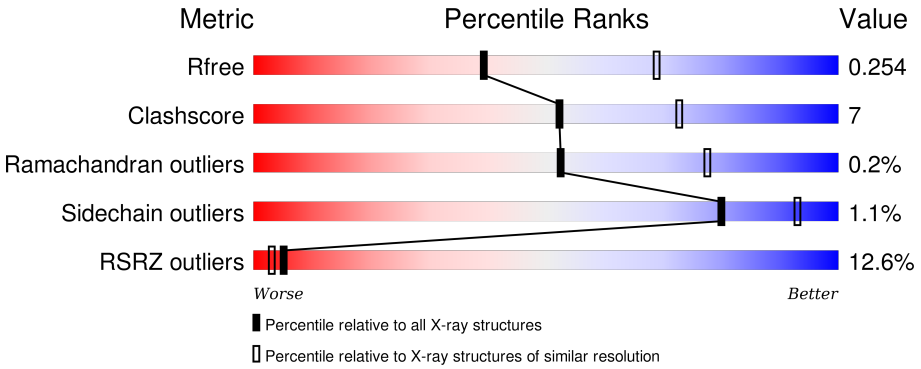
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 <=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	1030	10% 67% 12% • 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13444 atoms, of which 6655 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 Transcription elongation factor SPT6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	826	Total	C	H	N	O	S	0	0	0
			13396	4272	6655	1134	1317	18			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	GLY	-	EXPRESSION TAG	UNP P23615
A	231	ILE	-	EXPRESSION TAG	UNP P23615
A	232	ASP	-	EXPRESSION TAG	UNP P23615
A	233	PRO	-	EXPRESSION TAG	UNP P23615
A	234	PHE	-	EXPRESSION TAG	UNP P23615

- Molecule 2 is water.

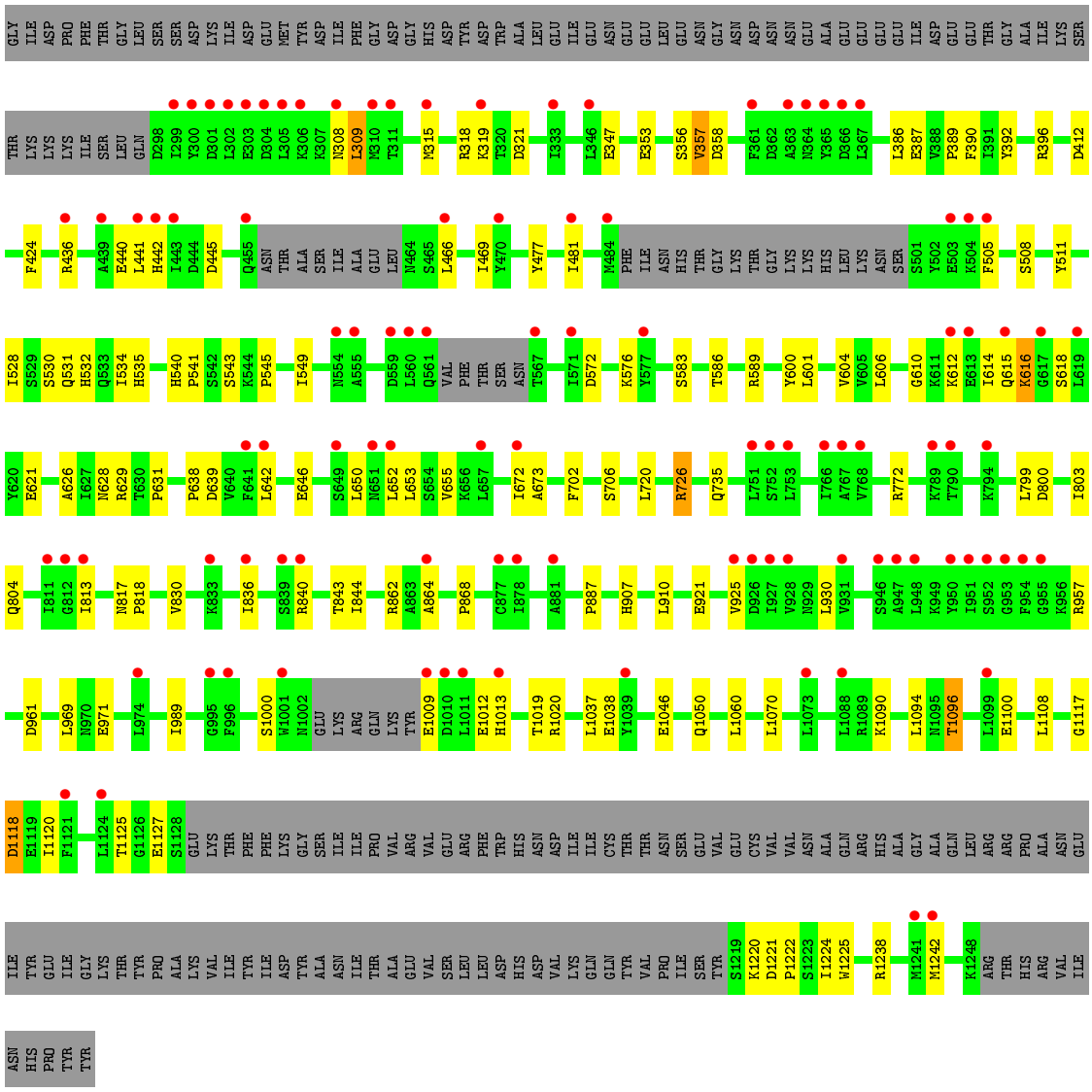
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	48	Total	O	0	0
			48	48		

3 Residue-property plots (i)

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: Transcription elongation factor SPT6

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	115.05Å 116.18Å 117.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.32 – 2.59 32.32 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.5 (32.32-2.59) 96.0 (32.32-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.224 , 0.265 0.207 , 0.254	Depositor DCC
R_{free} test set	1918 reflections (4.00%)	DCC
Wilson B-factor (Å^2)	65.1	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 56.3	EDS
Estimated twinning fraction	0.020 for -h,l,k 0.017 for -l,-k,-h 0.016 for k,h,-l 0.007 for k,l,h 0.007 for l,h,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 49536 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13444	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.33	0/6869	0.48	0/9278

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

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	6741	6655	6635	89	0
2	A	48	0	0	2	0
All	All	6789	6655	6635	89	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 7.

All (89) 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:A:626:ALA:HB1	1:A:629:ARG:HE	1.60	0.65
1:A:532:HIS:NE2	1:A:534:ILE:HG22	2.15	0.61
1:A:357:VAL:HG12	1:A:358:ASP:N	2.16	0.60
1:A:412:ASP:OD1	1:A:726:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:ASN:HB2	1:A:818:PRO:CD	2.33	0.58
1:A:615:GLN:O	1:A:616:LYS:HB2	2.04	0.58
1:A:1009:GLU:N	1:A:1012:GLU:HG2	2.19	0.58
1:A:615:GLN:O	1:A:616:LYS:CB	2.51	0.57
1:A:629:ARG:NH1	1:A:1224:ILE:HB	2.18	0.57
1:A:347:GLU:HB2	1:A:424:PHE:CE2	2.39	0.57
1:A:1046:GLU:O	1:A:1050:GLN:HG2	2.05	0.57
1:A:817:ASN:HB2	1:A:818:PRO:HD2	1.88	0.56
1:A:347:GLU:HG3	1:A:424:PHE:CG	2.41	0.56
1:A:650:LEU:HB3	1:A:652:LEU:HD13	1.90	0.54
1:A:604:VAL:HG13	1:A:653:LEU:HD22	1.90	0.53
1:A:803:ILE:HG21	1:A:836:ILE:HG21	1.91	0.53
1:A:530:SER:O	1:A:531:GLN:HB2	2.09	0.53
1:A:638:PRO:HB3	1:A:720:LEU:HD12	1.90	0.52
1:A:800:ASP:O	1:A:804:GLN:HG2	2.10	0.52
1:A:534:ILE:HG13	1:A:535:HIS:CD2	2.45	0.51
1:A:610:GLY:O	1:A:614:ILE:HG12	2.10	0.51
1:A:735:GLN:HB3	1:A:887:PRO:HG2	1.91	0.51
1:A:347:GLU:HG3	1:A:424:PHE:CD2	2.46	0.51
1:A:655:VAL:HG13	1:A:655:VAL:O	2.10	0.51
1:A:1019:THR:HB	1:A:1100:GLU:HB3	1.91	0.50
1:A:864:ALA:O	1:A:868:PRO:HA	2.12	0.50
1:A:604:VAL:CG1	1:A:653:LEU:HD22	2.42	0.49
1:A:612:LYS:O	1:A:615:GLN:HG2	2.12	0.49
1:A:441:LEU:HD21	1:A:481:ILE:HG22	1.94	0.49
1:A:642:LEU:HB2	1:A:910:LEU:HD13	1.95	0.49
1:A:511:TYR:O	1:A:511:TYR:CD2	2.66	0.49
1:A:1118:ASP:OD1	1:A:1118:ASP:N	2.45	0.49
1:A:392:TYR:CE2	1:A:396:ARG:NH2	2.82	0.48
1:A:1090:LYS:O	1:A:1094:LEU:HG	2.14	0.48
1:A:969:LEU:O	1:A:971:GLU:HG2	2.13	0.47
1:A:646:GLU:O	1:A:650:LEU:HG	2.15	0.47
1:A:650:LEU:CB	1:A:652:LEU:HD13	2.44	0.47
1:A:545:PRO:O	1:A:549:ILE:HG12	2.14	0.47
1:A:1117:GLY:HA2	1:A:1120:ILE:HD12	1.98	0.46
1:A:843:THR:HG22	2:A:29:HOH:O	2.14	0.46
1:A:642:LEU:CB	1:A:910:LEU:HD13	2.46	0.46
1:A:572:ASP:O	1:A:576:LYS:HG3	2.16	0.46
1:A:583:SER:O	1:A:589:ARG:HD2	2.15	0.46
1:A:1096:THR:O	1:A:1100:GLU:HG2	2.16	0.46
1:A:600:TYR:CE1	1:A:631:PRO:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:THR:HG22	1:A:1127:GLU:H	1.81	0.45
1:A:639:ASP:HB2	1:A:907:HIS:NE2	2.32	0.45
1:A:441:LEU:O	1:A:442:HIS:HB3	2.16	0.45
1:A:1221:ASP:OD1	1:A:1222:PRO:HD2	2.16	0.45
1:A:318:ARG:HD3	1:A:961:ASP:HB2	1.98	0.45
1:A:436:ARG:O	1:A:440:GLU:HB2	2.16	0.45
1:A:445:ASP:HB2	1:A:477:TYR:OH	2.17	0.45
1:A:1037:LEU:HD21	1:A:1060:LEU:HD12	1.98	0.45
1:A:799:LEU:HD23	1:A:830:VAL:HG11	1.99	0.44
1:A:702:PHE:O	1:A:706:SER:HB2	2.18	0.44
1:A:308:ASN:O	1:A:309:LEU:HB2	2.18	0.44
1:A:601:LEU:HB3	1:A:628:ASN:HA	1.97	0.44
1:A:353:GLU:O	1:A:356:SER:HB3	2.17	0.44
1:A:540:HIS:HD2	1:A:543:SER:H	1.66	0.44
1:A:650:LEU:O	1:A:652:LEU:HD12	2.18	0.44
1:A:1020:ARG:NH2	1:A:1108:LEU:HG	2.32	0.44
1:A:772:ARG:CZ	1:A:772:ARG:HB2	2.49	0.43
1:A:930:LEU:O	1:A:1020:ARG:NH1	2.52	0.43
1:A:386:LEU:HD13	1:A:390:PHE:CE2	2.54	0.43
1:A:1125:THR:CG2	1:A:1127:GLU:HG3	2.50	0.42
1:A:799:LEU:HD23	1:A:830:VAL:CG1	2.49	0.42
1:A:505:PHE:O	1:A:508:SER:HB3	2.18	0.42
1:A:653:LEU:HD12	1:A:653:LEU:C	2.40	0.42
1:A:836:ILE:HG22	1:A:844:ILE:HD12	2.00	0.42
1:A:1060:LEU:HD21	1:A:1070:LEU:HD11	2.02	0.42
1:A:540:HIS:HA	1:A:541:PRO:HD3	1.91	0.42
1:A:390:PHE:CD2	1:A:390:PHE:C	2.92	0.42
1:A:1238:ARG:NH1	1:A:1242:MET:SD	2.92	0.42
1:A:528:ILE:HG13	1:A:673:ALA:HB2	2.01	0.42
1:A:639:ASP:HB2	1:A:907:HIS:CD2	2.54	0.42
1:A:321:ASP:OD1	1:A:989:ILE:HG12	2.19	0.42
1:A:1037:LEU:O	1:A:1038:GLU:HB2	2.19	0.42
1:A:1220:LYS:HA	1:A:1225:TRP:CG	2.54	0.42
1:A:315:MET:O	1:A:319:LYS:HG2	2.20	0.42
1:A:621:GLU:O	1:A:621:GLU:HG2	2.20	0.42
1:A:862:ARG:NH2	2:A:47:HOH:O	2.53	0.41
1:A:387:GLU:HB3	1:A:389:PRO:HD2	2.01	0.41
1:A:672:ILE:CG2	1:A:672:ILE:O	2.67	0.41
1:A:606:LEU:HD23	1:A:653:LEU:HB3	2.03	0.41
1:A:309:LEU:HB3	1:A:957:ARG:HG2	2.03	0.41
1:A:469:ILE:HD13	1:A:586:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:921:GLU:O	1:A:925:VAL:HG23	2.21	0.40
1:A:840:ARG:O	1:A:840:ARG:HG3	2.21	0.40
1:A:466:LEU:HD12	1:A:466:LEU:HA	1.96	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	814/1030 (79%)	772 (95%)	40 (5%)	2 (0%)	52 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	616	LYS
1	A	357	VAL

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	748/929 (80%)	740 (99%)	8 (1%)	80 93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	LEU
1	A	618	SER
1	A	726	ARG
1	A	813	ILE
1	A	1000	SER
1	A	1013	HIS
1	A	1096	THR
1	A	1118	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	HIS
1	A	535	HIS
1	A	540	HIS
1	A	575	GLN
1	A	885	HIS
1	A	1013	HIS

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

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, 95^{th} 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	826/1030 (80%)	0.81	104 (12%) 5 3	57, 89, 148, 201	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1011	LEU	6.2
1	A	560	LEU	6.1
1	A	481	ILE	5.9
1	A	504	LYS	5.9
1	A	649	SER	5.7
1	A	302	LEU	5.3
1	A	1010	ASP	5.1
1	A	299	ILE	5.1
1	A	300	TYR	5.1
1	A	442	HIS	5.0
1	A	839	SER	4.9
1	A	365	TYR	4.7
1	A	651	ASN	4.7
1	A	652	LEU	4.6
1	A	303	GLU	4.3
1	A	305	LEU	4.2
1	A	1009	GLU	4.2
1	A	619	LEU	4.2
1	A	304	ASP	4.2
1	A	615	GLN	4.1
1	A	1124	LEU	3.9
1	A	436	ARG	3.7
1	A	1242	MET	3.7
1	A	319	LYS	3.6
1	A	571	ILE	3.5
1	A	840	ARG	3.4
1	A	951	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	363	ALA	3.4
1	A	310	MET	3.4
1	A	877	CYS	3.3
1	A	364	ASN	3.2
1	A	953	GLY	3.2
1	A	952	SER	3.2
1	A	1121	PHE	3.1
1	A	751	LEU	3.1
1	A	813	ILE	3.1
1	A	561	GLN	3.1
1	A	443	ILE	3.1
1	A	790	THR	3.0
1	A	767	ALA	3.0
1	A	554	ASN	2.9
1	A	974	LEU	2.9
1	A	752	SER	2.9
1	A	346	LEU	2.8
1	A	864	ALA	2.8
1	A	641	PHE	2.8
1	A	836	ILE	2.8
1	A	505	PHE	2.8
1	A	768	VAL	2.8
1	A	928	VAL	2.8
1	A	1073	LEU	2.8
1	A	878	ILE	2.7
1	A	789	LYS	2.7
1	A	833	LYS	2.7
1	A	301	ASP	2.7
1	A	555	ALA	2.7
1	A	470	TYR	2.7
1	A	927	ILE	2.6
1	A	315	MET	2.6
1	A	947	ALA	2.6
1	A	466	LEU	2.6
1	A	881	ALA	2.6
1	A	954	PHE	2.6
1	A	455	GLN	2.5
1	A	955	GLY	2.5
1	A	361	PHE	2.5
1	A	1001	TRP	2.5
1	A	1039	TYR	2.5
1	A	612	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	366	ASP	2.4
1	A	503	GLU	2.4
1	A	1241	MET	2.4
1	A	753	LEU	2.4
1	A	567	THR	2.4
1	A	946	SER	2.4
1	A	333	ILE	2.4
1	A	484	MET	2.4
1	A	306	LYS	2.3
1	A	367	LEU	2.3
1	A	950	TYR	2.2
1	A	766	ILE	2.2
1	A	642	LEU	2.2
1	A	794	LYS	2.2
1	A	812	GLY	2.2
1	A	439	ALA	2.2
1	A	931	VAL	2.1
1	A	995	GLY	2.1
1	A	672	ILE	2.1
1	A	559	ASP	2.1
1	A	657	LEU	2.1
1	A	948	LEU	2.1
1	A	308	ASN	2.1
1	A	1013	HIS	2.1
1	A	996	PHE	2.1
1	A	441	LEU	2.1
1	A	1099	LEU	2.1
1	A	613	GLU	2.1
1	A	1088	LEU	2.1
1	A	925	VAL	2.0
1	A	617	GLY	2.0
1	A	926	ASP	2.0
1	A	811	ILE	2.0
1	A	311	THR	2.0
1	A	577	TYR	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

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.