



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:46 pm GMT

PDB ID : 5ESY  
Title : Arabidopsis thaliana SAL1  
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Deposited on : 2015-11-17  
Resolution : 3.05 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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

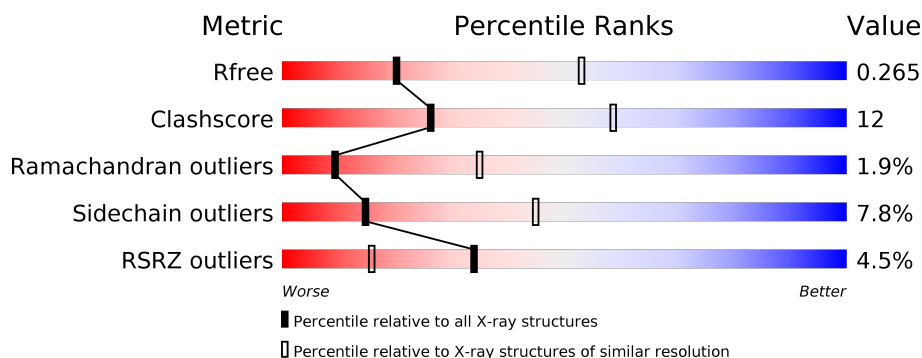
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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))
$R_{free}$	100719	1348 (3.10-3.02)
Clashscore	112137	1462 (3.10-3.02)
Ramachandran outliers	110173	1410 (3.10-3.02)
Sidechain outliers	110143	1410 (3.10-3.02)
RSRZ outliers	101464	1355 (3.10-3.02)

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	346	<div> <div>6%</div> <div>67%</div> <div>31%</div> <div>•</div> </div>
1	B	346	<div> <div>3%</div> <div>71%</div> <div>27%</div> <div>•</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5082 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.

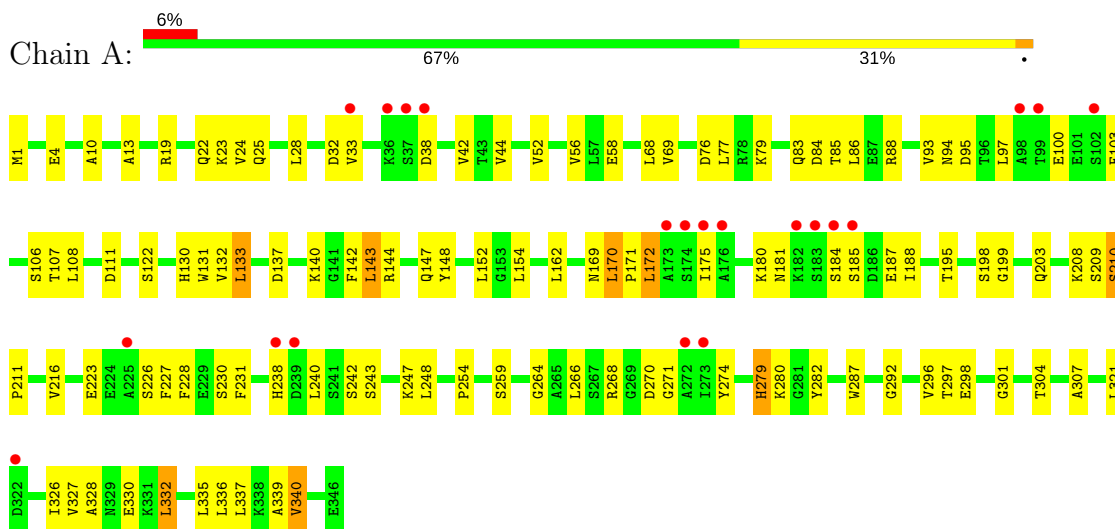
- Molecule 1 is a protein called SAL1 phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2544	1592	426	520	6			
1	B	346	Total	C	N	O	S	0	0	0
			2538	1593	425	513	7			

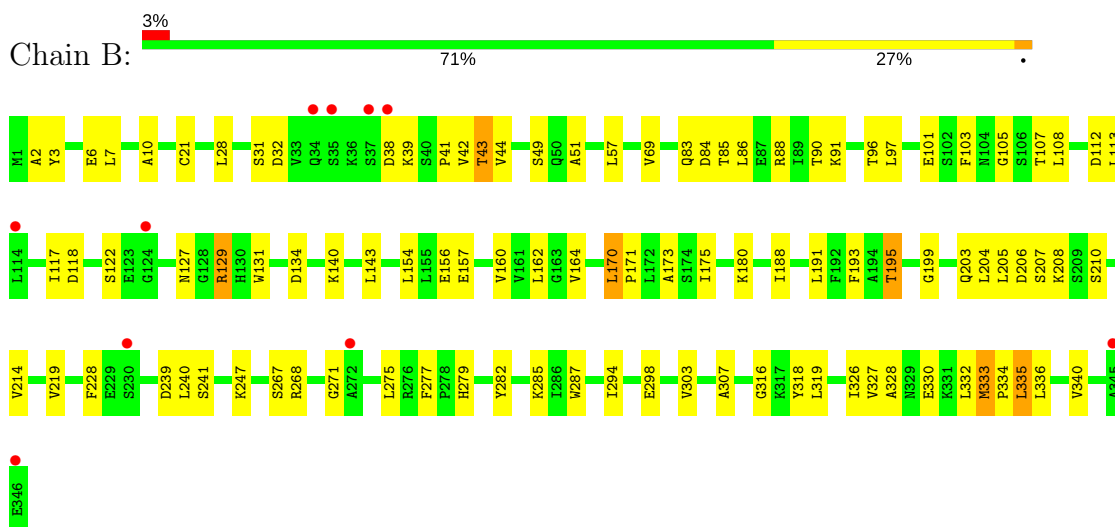
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: SAL1 phosphatase



- Molecule 1: SAL1 phosphatase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.14Å 137.14Å 74.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.47 – 3.05 38.47 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.47-3.05) 95.7 (38.47-3.05)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 3.06Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.228 , 0.265 0.228 , 0.265	Depositor DCC
$R_{free}$ test set	825 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.6	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.467 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.490 for h,-h-k,-l	Depositor
Outliers	0 of 15324 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5082	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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, 0.333 respectively for untwinned datasets, and 0.375, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.25	0/2581	0.52	0/3498
1	B	0.25	0/2575	0.51	0/3490
All	All	0.25	0/5156	0.52	0/6988

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	2544	0	2510	64	1
1	B	2538	0	2510	55	1
All	All	5082	0	5020	118	1

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 12.

All (118) 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:268:ARG:NH2	1:A:270:ASP:OD2	2.23	0.71
1:B:154:LEU:HB3	1:B:162:LEU:HG	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ALA:HA	1:B:340:VAL:HG11	1.76	0.67
1:A:22:GLN:O	1:A:25:GLN:NE2	2.28	0.67
1:B:31:SER:OG	1:B:32:ASP:N	2.29	0.66
1:A:143:LEU:HD23	1:A:144:ARG:H	1.62	0.65
1:B:275:LEU:HD22	1:B:326:ILE:HG22	1.78	0.65
1:B:175:ILE:HD11	1:B:180:LYS:HB3	1.79	0.64
1:A:199:GLY:HA2	1:A:298:GLU:HB3	1.81	0.63
1:A:336:LEU:O	1:A:340:VAL:N	2.32	0.63
1:B:21:CYS:SG	1:B:49:SER:OG	2.57	0.62
1:A:195:THR:HG23	1:A:198:SER:HB2	1.81	0.61
1:A:147:GLN:NE2	1:A:169:ASN:O	2.31	0.61
1:B:275:LEU:HB3	1:B:277:PHE:HE1	1.65	0.60
1:B:162:LEU:HB3	1:B:195:THR:HG23	1.84	0.60
1:B:239:ASP:C	1:B:241:SER:H	2.05	0.59
1:B:86:LEU:HB3	1:B:113:LEU:HG	1.85	0.58
1:B:134:ASP:HB2	1:B:287:TRP:HB2	1.85	0.58
1:A:328:ALA:HB2	1:A:336:LEU:HD13	1.87	0.56
1:A:10:ALA:HB1	1:A:152:LEU:HD11	1.86	0.56
1:A:83:GLN:HA	1:A:86:LEU:HD13	1.88	0.56
1:A:279:HIS:O	1:A:280:LYS:HG2	2.06	0.56
1:A:240:LEU:HB3	1:A:243:SER:HB3	1.88	0.56
1:A:170:LEU:N	1:A:188:ILE:O	2.29	0.56
1:B:156:GLU:HG2	1:B:157:GLU:HG2	1.87	0.56
1:A:332:LEU:HD12	1:A:335:LEU:HB3	1.87	0.56
1:B:333:MET:HG3	1:B:334:PRO:HD3	1.88	0.55
1:A:280:LYS:HG3	1:A:282:TYR:H	1.71	0.55
1:B:204:LEU:HB3	1:B:207:SER:O	2.07	0.55
1:B:90:THR:OG1	1:B:91:LYS:N	2.40	0.55
1:B:188:ILE:HB	1:B:204:LEU:HD11	1.89	0.54
1:A:97:LEU:HD22	1:A:107:THR:HB	1.89	0.54
1:A:1:MET:N	1:A:4:GLU:OE2	2.37	0.54
1:B:328:ALA:HB3	1:B:336:LEU:HD11	1.89	0.54
1:A:94:ASN:ND2	1:A:95:ASP:OD1	2.41	0.54
1:B:282:TYR:OH	1:B:285:LYS:NZ	2.25	0.54
1:A:169:ASN:HA	1:A:188:ILE:HG22	1.89	0.54
1:A:69:VAL:N	1:A:131:TRP:O	2.42	0.53
1:B:239:ASP:O	1:B:241:SER:N	2.42	0.53
1:A:111:ASP:N	1:A:111:ASP:OD1	2.40	0.53
1:A:335:LEU:HD12	1:A:337:LEU:H	1.74	0.53
1:B:275:LEU:HB3	1:B:277:PHE:CE1	2.43	0.53
1:A:336:LEU:HA	1:A:339:ALA:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:VAL:O	1:A:56:VAL:HG12	2.10	0.52
1:B:332:LEU:HB3	1:B:335:LEU:HD23	1.92	0.51
1:B:193:PHE:HE1	1:B:203:GLN:HB2	1.77	0.50
1:B:69:VAL:N	1:B:131:TRP:O	2.43	0.50
1:A:42:VAL:HB	1:A:44:VAL:HG23	1.95	0.49
1:A:147:GLN:HG3	1:A:259:SER:HB2	1.93	0.49
1:A:240:LEU:HG	1:A:242:SER:H	1.76	0.49
1:A:172:LEU:HD13	1:A:172:LEU:H	1.77	0.48
1:B:336:LEU:HD12	1:B:336:LEU:H	1.79	0.48
1:B:10:ALA:HA	1:B:57:LEU:HD21	1.96	0.48
1:B:330:GLU:O	1:B:333:MET:HB3	2.14	0.47
1:A:274:TYR:HB3	1:A:327:VAL:HB	1.96	0.47
1:B:38:ASP:OD1	1:B:39:LYS:N	2.42	0.47
1:A:68:LEU:HD11	1:A:133:LEU:HD22	1.95	0.47
1:B:173:ALA:H	1:B:268:ARG:NH2	2.13	0.47
1:B:160:VAL:HG22	1:B:294:ILE:HD11	1.97	0.47
1:A:23:LYS:HD2	1:A:23:LYS:HA	1.61	0.47
1:A:154:LEU:HB3	1:A:162:LEU:HG	1.97	0.47
1:A:307:ALA:HA	1:A:337:LEU:HD22	1.96	0.47
1:B:199:GLY:HA2	1:B:298:GLU:HB3	1.98	0.46
1:A:140:LYS:O	1:A:143:LEU:HD22	2.16	0.46
1:B:228:PHE:HE1	1:B:271:GLY:HA3	1.78	0.46
1:B:303:VAL:HG22	1:B:327:VAL:HG22	1.97	0.46
1:A:76:ASP:N	1:A:76:ASP:OD1	2.48	0.46
1:B:3:TYR:HB3	1:B:6:GLU:HB2	1.97	0.45
1:A:326:ILE:HB	1:A:336:LEU:HD22	1.98	0.45
1:A:144:ARG:HD2	1:A:144:ARG:HA	1.72	0.45
1:A:226:SER:HB2	1:A:271:GLY:HA2	1.98	0.45
1:B:84:ASP:OD1	1:B:85:THR:N	2.49	0.45
1:B:303:VAL:HG13	1:B:327:VAL:HG22	1.99	0.45
1:A:84:ASP:O	1:A:88:ARG:HG2	2.16	0.45
1:A:97:LEU:HD21	1:A:106:SER:N	2.31	0.44
1:B:160:VAL:CG2	1:B:294:ILE:HD11	2.47	0.44
1:A:19:ARG:NH2	1:A:93:VAL:HG11	2.32	0.44
1:A:335:LEU:HB2	1:A:336:LEU:H	1.55	0.44
1:A:84:ASP:OD1	1:A:85:THR:N	2.48	0.44
1:B:129:ARG:HG2	1:B:154:LEU:HD11	1.98	0.44
1:B:108:LEU:O	1:B:112:ASP:HB2	2.18	0.44
1:B:239:ASP:C	1:B:241:SER:N	2.71	0.43
1:B:205:LEU:O	1:B:207:SER:N	2.49	0.43
1:B:214:VAL:HB	1:B:267:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ALA:HA	1:A:56:VAL:HG11	2.00	0.43
1:B:96:THR:O	1:B:105:GLY:HA3	2.19	0.43
1:A:148:TYR:HA	1:A:259:SER:OG	2.18	0.43
1:A:297:THR:HA	1:A:301:GLY:O	2.19	0.43
1:A:38:ASP:OD1	1:A:38:ASP:N	2.40	0.43
1:A:24:VAL:O	1:A:25:GLN:NE2	2.52	0.42
1:A:264:GLY:O	1:A:268:ARG:N	2.50	0.42
1:B:90:THR:O	1:B:108:LEU:HD21	2.17	0.42
1:A:185:SER:O	1:A:187:GLU:N	2.44	0.42
1:A:228:PHE:HB2	1:A:274:TYR:HD1	1.83	0.42
1:B:140:LYS:HD2	1:B:143:LEU:HD22	2.01	0.42
1:A:198:SER:OG	1:B:2:ALA:HA	2.19	0.42
1:B:333:MET:HG3	1:B:334:PRO:CD	2.50	0.42
1:A:171:PRO:HB3	1:A:185:SER:HB3	2.02	0.42
1:A:210:SER:HA	1:A:211:PRO:HD2	1.72	0.42
1:B:239:ASP:HA	1:B:279:HIS:NE2	2.35	0.42
1:A:140:LYS:HA	1:A:140:LYS:HD3	1.80	0.42
1:B:7:LEU:HD11	1:B:193:PHE:HB2	2.01	0.42
1:B:88:ARG:HD3	1:B:88:ARG:HA	1.76	0.41
1:A:240:LEU:O	1:A:243:SER:OG	2.34	0.41
1:A:79:LYS:HD3	1:A:79:LYS:HA	1.78	0.41
1:A:216:VAL:HG21	1:A:301:GLY:N	2.36	0.41
1:A:77:LEU:HA	1:A:77:LEU:HD12	1.85	0.41
1:B:42:VAL:HG22	1:B:44:VAL:HG23	2.02	0.41
1:B:51:ALA:HB2	1:B:117:ILE:HD11	2.02	0.41
1:B:43:THR:OG1	1:B:43:THR:O	2.38	0.41
1:A:227:PHE:HB2	1:A:254:PRO:HB3	2.02	0.41
1:A:132:VAL:HG12	1:A:287:TRP:HB3	2.02	0.41
1:B:170:LEU:HA	1:B:171:PRO:HD2	1.91	0.41
1:B:316:GLY:O	1:B:318:TYR:N	2.45	0.41
1:A:203:GLN:NE2	1:A:208:LYS:HA	2.37	0.40
1:A:292:GLY:O	1:A:296:VAL:HG22	2.22	0.40
1:B:164:VAL:HG13	1:B:191:LEU:HD11	2.03	0.40
1:A:38:ASP:OD2	1:A:42:VAL:HG13	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:SER:OG	1:B:206:ASP:OD2[4_665]	2.15	0.05

## 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	344/346 (99%)	291 (85%)	47 (14%)	6 (2%)	11	38
1	B	344/346 (99%)	298 (87%)	39 (11%)	7 (2%)	9	33
All	All	688/692 (99%)	589 (86%)	86 (12%)	13 (2%)	9	35

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	219	VAL
1	A	100	GLU
1	A	122	SER
1	A	231	PHE
1	B	43	THR
1	B	240	LEU
1	A	175	ILE
1	A	181	ASN
1	B	122	SER
1	B	210	SER
1	A	210	SER
1	B	101	GLU
1	B	41	PRO

### 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	272/282 (96%)	245 (90%)	27 (10%)	9	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	269/282 (95%)	254 (94%)	15 (6%)	25	58
All	All	541/564 (96%)	499 (92%)	42 (8%)	15	45

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	32	ASP
1	A	33	VAL
1	A	58	GLU
1	A	103	PHE
1	A	108	LEU
1	A	130	HIS
1	A	133	LEU
1	A	137	ASP
1	A	142	PHE
1	A	143	LEU
1	A	170	LEU
1	A	172	LEU
1	A	180	LYS
1	A	184	SER
1	A	223	GLU
1	A	230	SER
1	A	238	HIS
1	A	247	LYS
1	A	248	LEU
1	A	266	LEU
1	A	279	HIS
1	A	304	THR
1	A	321	LEU
1	A	330	GLU
1	A	332	LEU
1	A	340	VAL
1	B	28	LEU
1	B	83	GLN
1	B	97	LEU
1	B	103	PHE
1	B	107	THR
1	B	118	ASP
1	B	127	ASN
1	B	129	ARG
1	B	170	LEU

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Mol	Chain	Res	Type
1	B	195	THR
1	B	208	LYS
1	B	247	LYS
1	B	319	LEU
1	B	333	MET
1	B	335	LEU

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

### 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	346/346 (100%)	-0.16	21 (6%) 22 9	47, 101, 189, 251	0
1	B	346/346 (100%)	-0.24	10 (2%) 52 27	47, 107, 163, 229	0
All	All	692/692 (100%)	-0.20	31 (4%) 34 16	47, 105, 174, 251	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	ALA	7.1
1	B	346	GLU	6.0
1	B	35	SER	5.6
1	A	37	SER	4.9
1	A	38	ASP	4.8
1	A	183	SER	4.7
1	A	184	SER	4.3
1	A	36	LYS	4.0
1	A	174	SER	4.0
1	A	175	ILE	3.7
1	B	230	SER	3.5
1	A	33	VAL	3.5
1	B	345	ALA	3.3
1	A	102	SER	3.3
1	A	239	ASP	3.1
1	A	182	LYS	3.0
1	A	185	SER	2.8
1	A	225	ALA	2.7
1	B	38	ASP	2.6
1	B	34	GLN	2.5
1	B	124	GLY	2.4
1	B	37	SER	2.4
1	A	238	HIS	2.3
1	A	272	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	272	ALA	2.2
1	B	114	LEU	2.2
1	A	173	ALA	2.1
1	A	273	ILE	2.1
1	A	98	ALA	2.1
1	A	99	THR	2.1
1	A	322	ASP	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 [i](#)

There are no carbohydrates 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.