



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:24 AM GMT

PDB ID : 2Q4E
Title : Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At4g09670
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-31
Resolution : 2.49 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 ⓘ symbol.

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

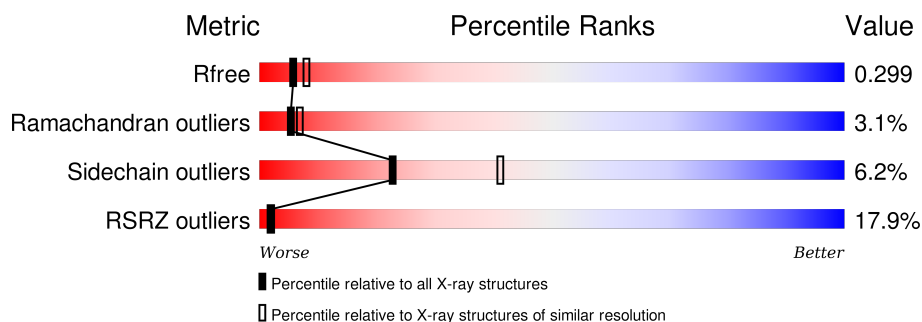
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	3553 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	1-A	362	<div> <div>22%</div> <div>87%</div> <div>7%</div> <div>5%</div> </div>
1	1-B	362	<div> <div>15%</div> <div>90%</div> <div>6%</div> <div>•</div> </div>
1	10-A	362	<div> <div>22%</div> <div>88%</div> <div>7%</div> <div>5%</div> </div>
1	10-B	362	<div> <div>15%</div> <div>91%</div> <div>6%</div> <div>•</div> </div>
1	11-A	362	<div> <div>22%</div> <div>88%</div> <div>6%</div> <div>5%</div> </div>
1	11-B	362	<div> <div>15%</div> <div>89%</div> <div>7%</div> <div>•</div> </div>
1	12-A	362	<div> <div>22%</div> <div>85%</div> <div>10%</div> <div>5%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	12-B	362	
1	13-A	362	
1	13-B	362	
1	14-A	362	
1	14-B	362	
1	15-A	362	
1	15-B	362	
1	16-A	362	
1	16-B	362	
1	2-A	362	
1	2-B	362	
1	3-A	362	
1	3-B	362	
1	4-A	362	
1	4-B	362	
1	5-A	362	
1	5-B	362	
1	6-A	362	
1	6-B	362	
1	7-A	362	
1	7-B	362	
1	8-A	362	
1	8-B	362	
1	9-A	362	
1	9-B	362	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 87408 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 Probable oxidoreductase At4g09670.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	2-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	3-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	4-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	5-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	6-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	7-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	8-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	9-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	10-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	11-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	12-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	13-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	14-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	15-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			
1	16-A	343	Total	C	N	O	S	Se	0	0	0
			2648	1687	445	504	6	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			
1	2-B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			
1	3-B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			
1	4-B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			
1	5-B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			
1	6-B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			
1	7-B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			
1	8-B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			
1	9-B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			
1	10-B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			
1	11-B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			
1	12-B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			
1	13-B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			
1	14-B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			
1	15-B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			
1	16-B	350	Total	C	N	O	S	Se	0	0	0
			2692	1712	453	515	6	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP Q9SZ83
A	12	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
A	106	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
A	126	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
A	130	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
A	249	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
A	310	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	SER	-	EXPRESSION TAG	UNP Q9SZ83
B	12	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
B	106	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
B	126	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
B	130	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
B	249	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83
B	310	MSE	MET	MODIFIED RESIDUE	UNP Q9SZ83

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	60	Total O 60 60	0	0
2	2-A	58	Total O 58 58	0	0
2	3-A	62	Total O 62 62	0	0
2	4-A	60	Total O 60 60	0	0
2	5-A	59	Total O 59 59	0	0
2	6-A	60	Total O 60 60	0	0
2	7-A	61	Total O 61 61	0	0
2	8-A	56	Total O 56 56	0	0
2	9-A	60	Total O 60 60	0	0
2	10-A	59	Total O 59 59	0	0
2	11-A	60	Total O 60 60	0	0
2	12-A	61	Total O 61 61	0	0
2	13-A	62	Total O 62 62	0	0
2	14-A	59	Total O 59 59	0	0
2	15-A	59	Total O 59 59	0	0
2	16-A	60	Total O 60 60	0	0

Continued on next page...

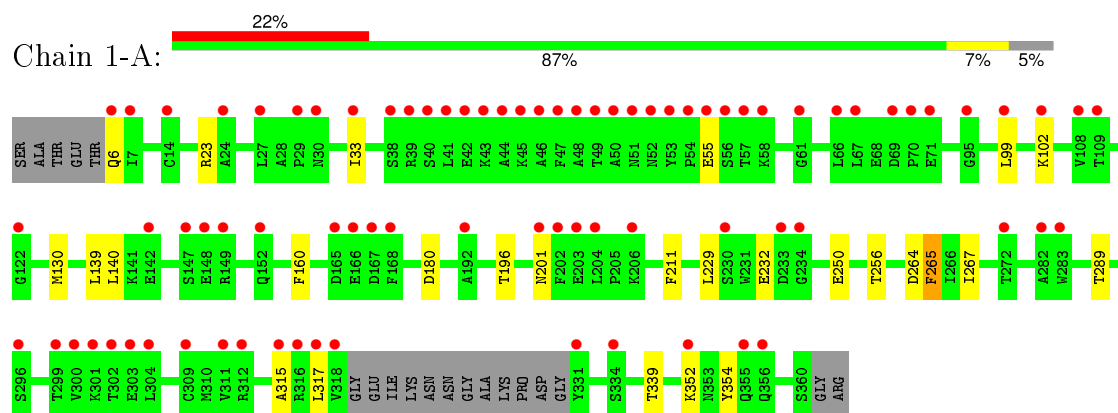
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-B	63	Total O 63 63	0	0
2	2-B	65	Total O 65 65	0	0
2	3-B	61	Total O 61 61	0	0
2	4-B	63	Total O 63 63	0	0
2	5-B	64	Total O 64 64	0	0
2	6-B	63	Total O 63 63	0	0
2	7-B	62	Total O 62 62	0	0
2	8-B	67	Total O 67 67	0	0
2	9-B	63	Total O 63 63	0	0
2	10-B	64	Total O 64 64	0	0
2	11-B	63	Total O 63 63	0	0
2	12-B	62	Total O 62 62	0	0
2	13-B	61	Total O 61 61	0	0
2	14-B	64	Total O 64 64	0	0
2	15-B	64	Total O 64 64	0	0
2	16-B	63	Total O 63 63	0	0

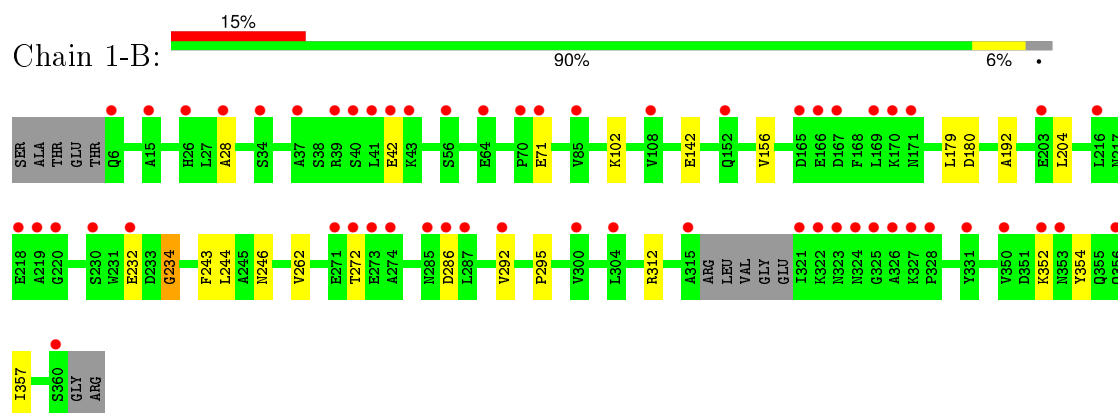
3 Residue-property plots [i](#)

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.

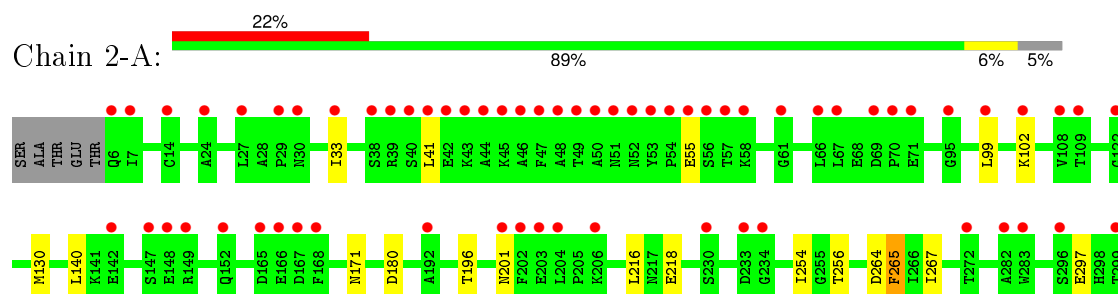
- Molecule 1: Probable oxidoreductase At4g09670



- Molecule 1: Probable oxidoreductase At4g09670

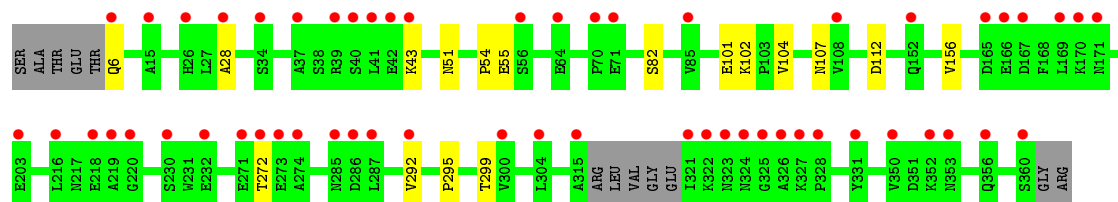


- Molecule 1: Probable oxidoreductase At4g09670

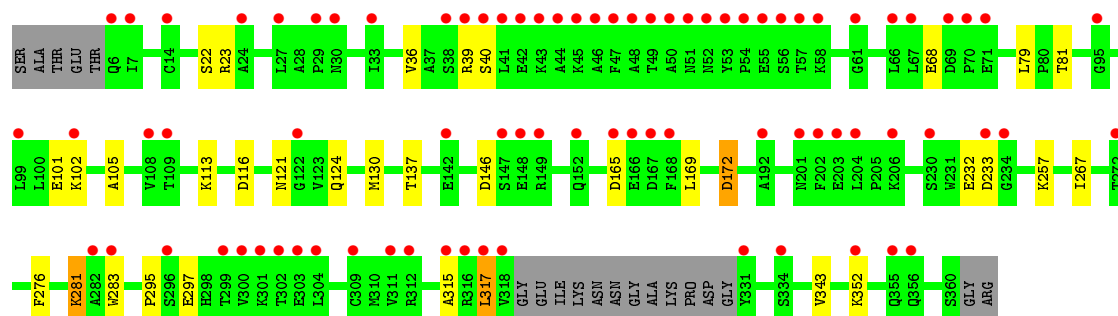
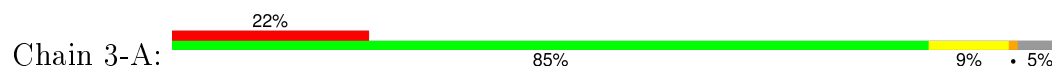




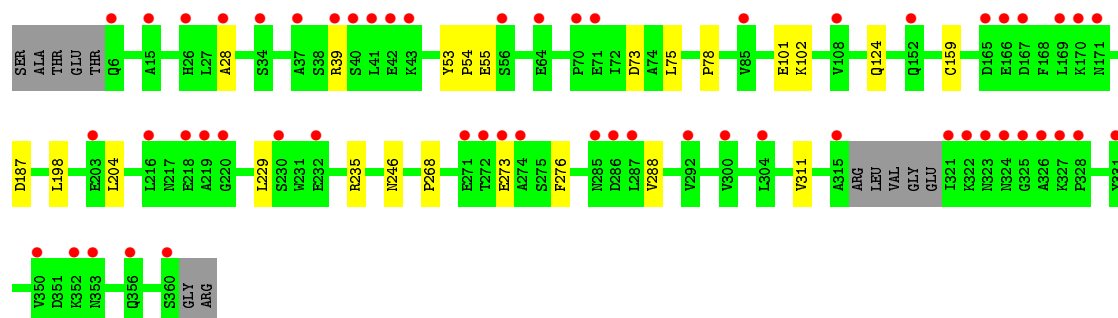
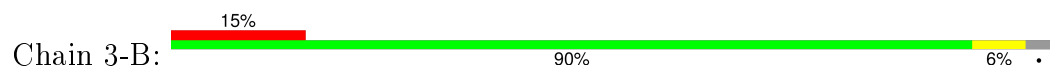
- Molecule 1: Probable oxidoreductase At4g09670



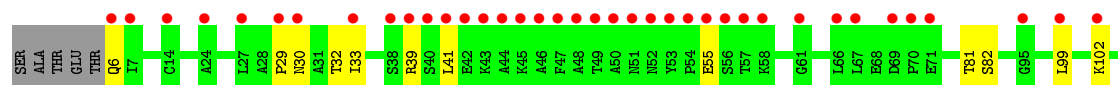
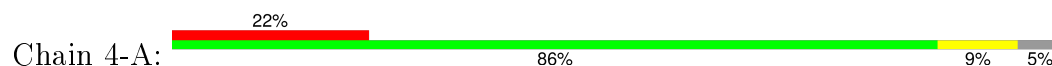
- Molecule 1: Probable oxidoreductase At4g09670

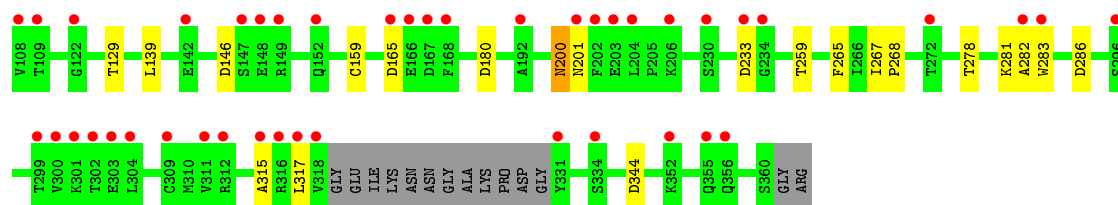


- Molecule 1: Probable oxidoreductase At4g09670

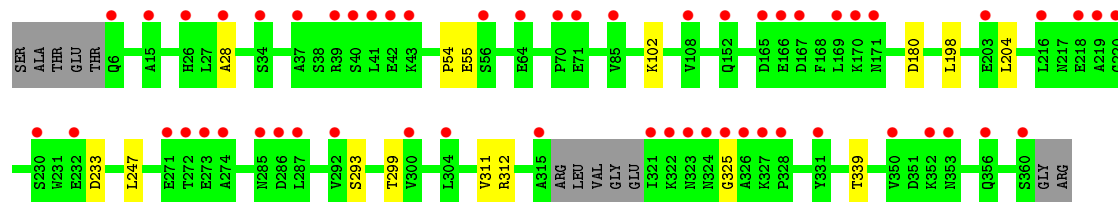


- Molecule 1: Probable oxidoreductase At4g09670

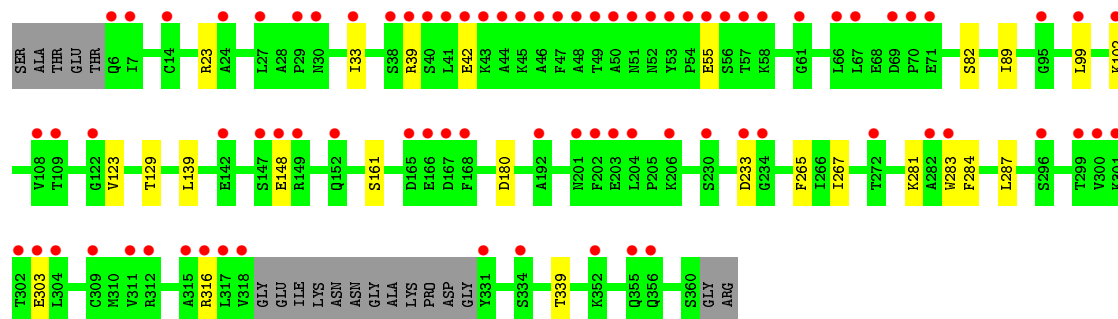
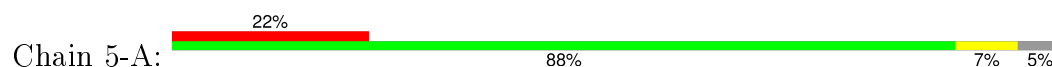




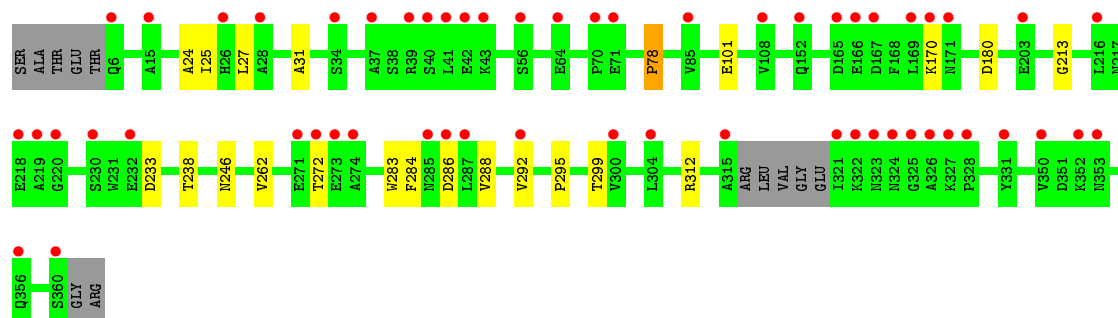
- Molecule 1: Probable oxidoreductase At4g09670



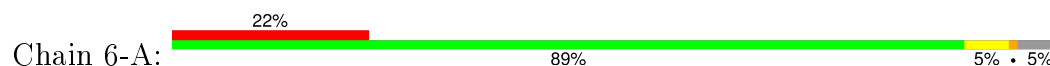
- Molecule 1: Probable oxidoreductase At4g09670

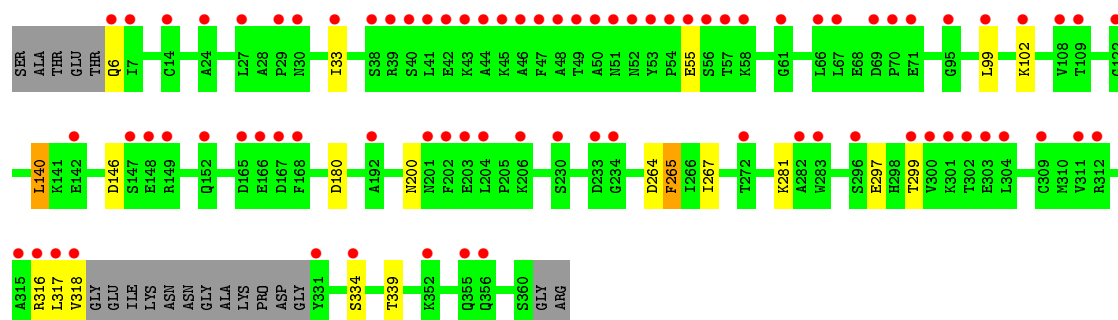


- Molecule 1: Probable oxidoreductase At4g09670

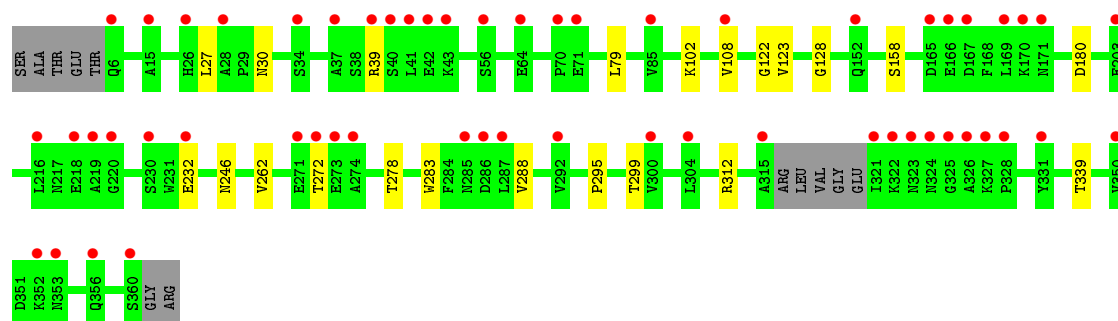


- Molecule 1: Probable oxidoreductase At4g09670

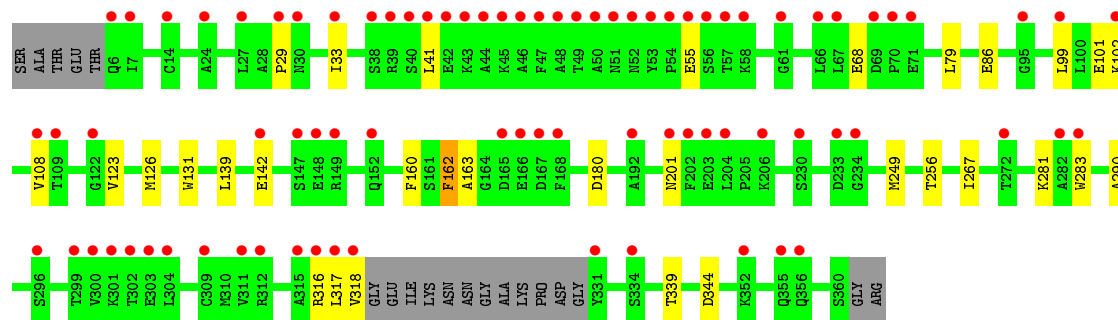
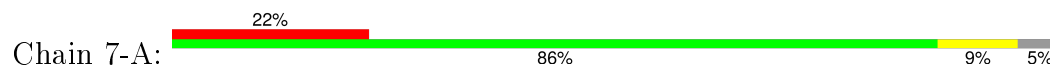




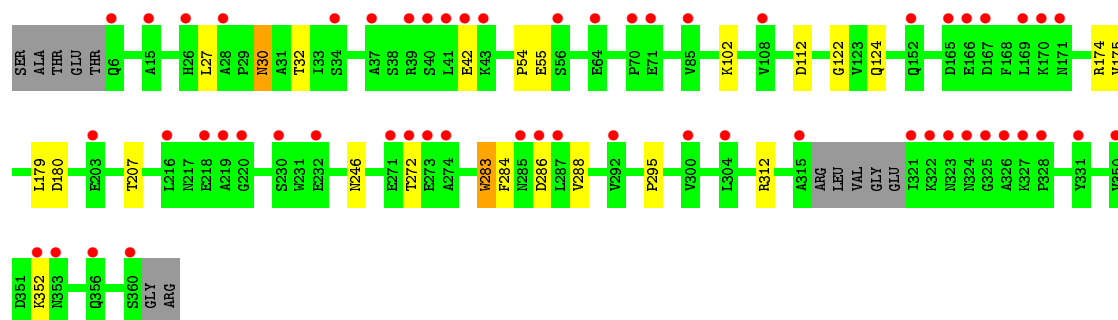
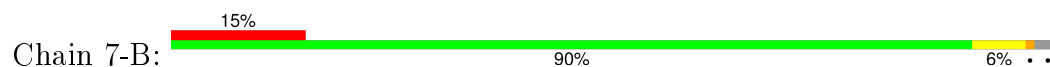
- Molecule 1: Probable oxidoreductase At4g09670



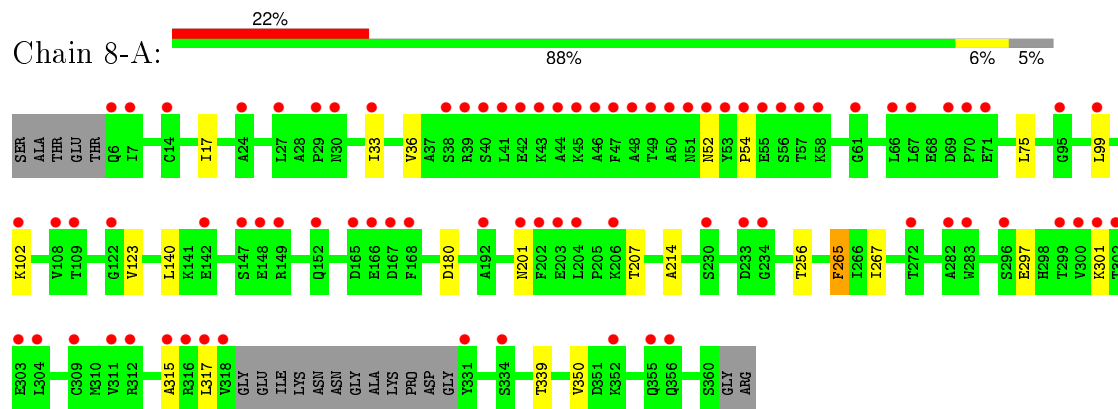
- Molecule 1: Probable oxidoreductase At4g09670



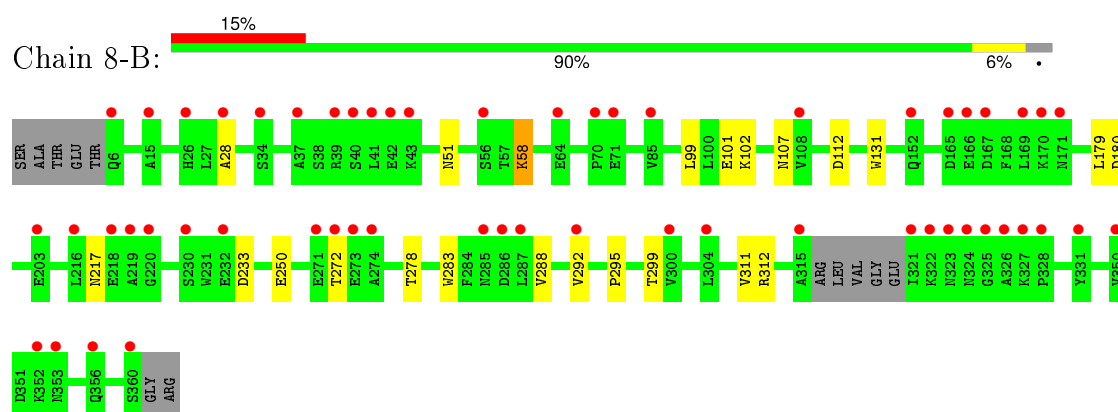
- Molecule 1: Probable oxidoreductase At4g09670



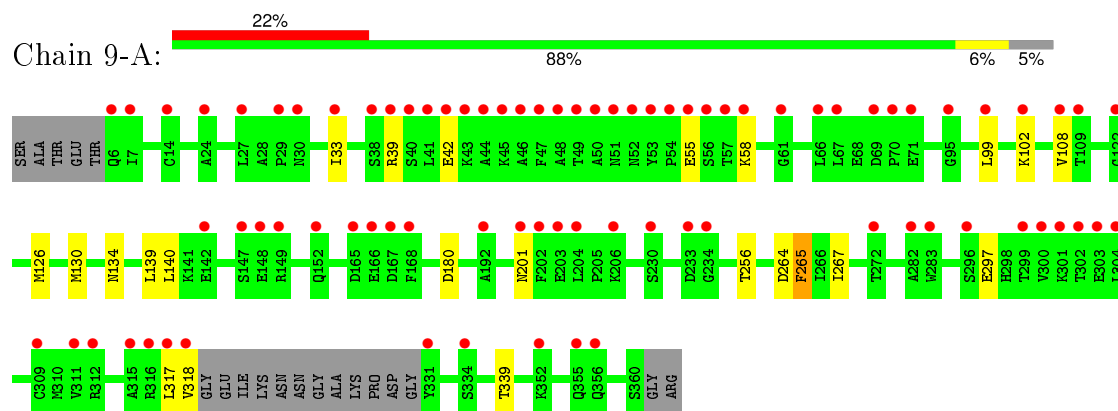
• Molecule 1: Probable oxidoreductase At4g09670



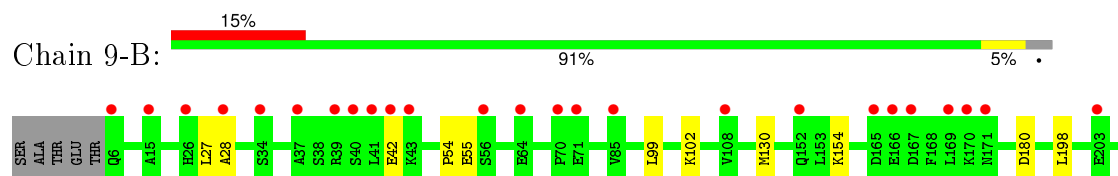
• Molecule 1: Probable oxidoreductase At4g09670

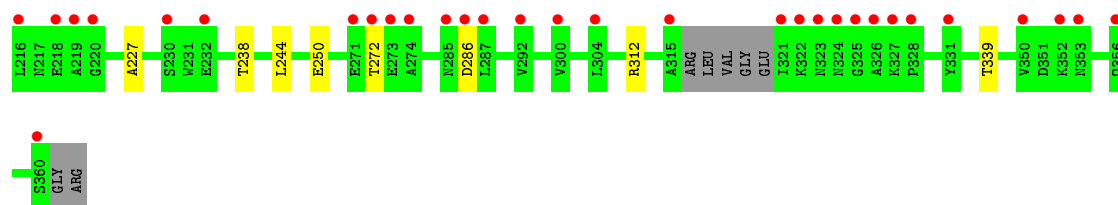


• Molecule 1: Probable oxidoreductase At4g09670

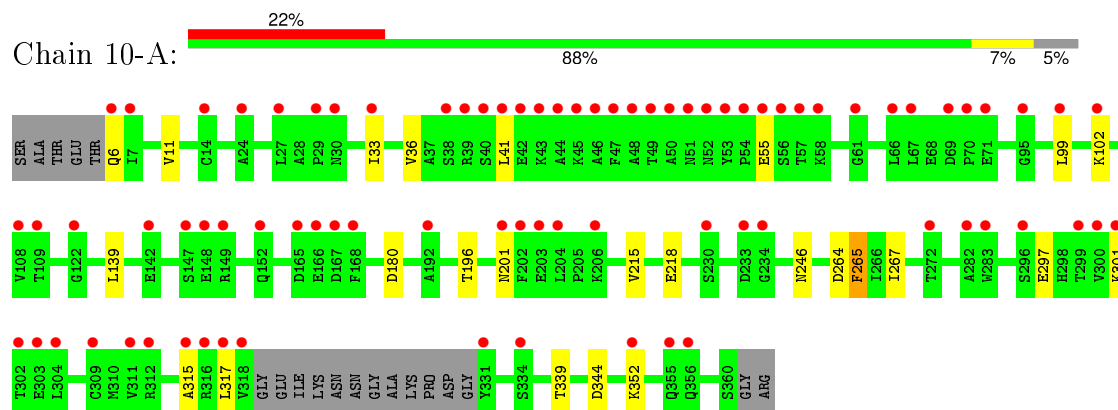


• Molecule 1: Probable oxidoreductase At4g09670

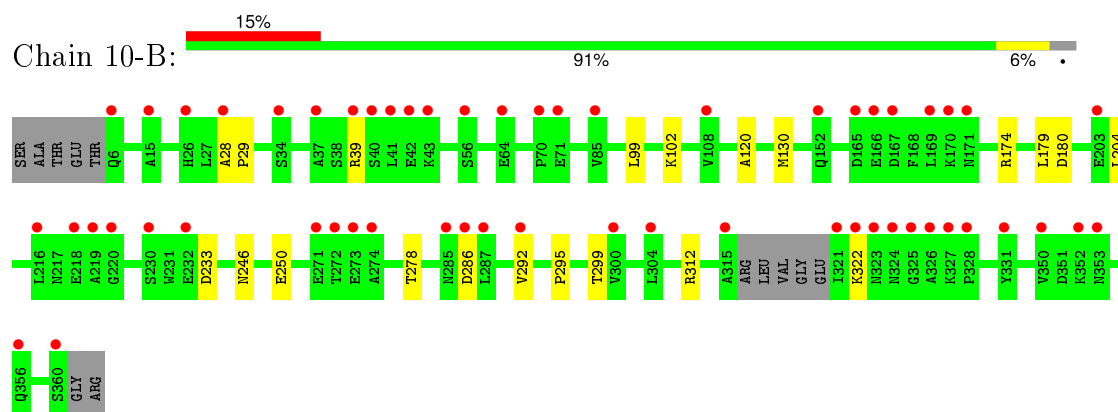




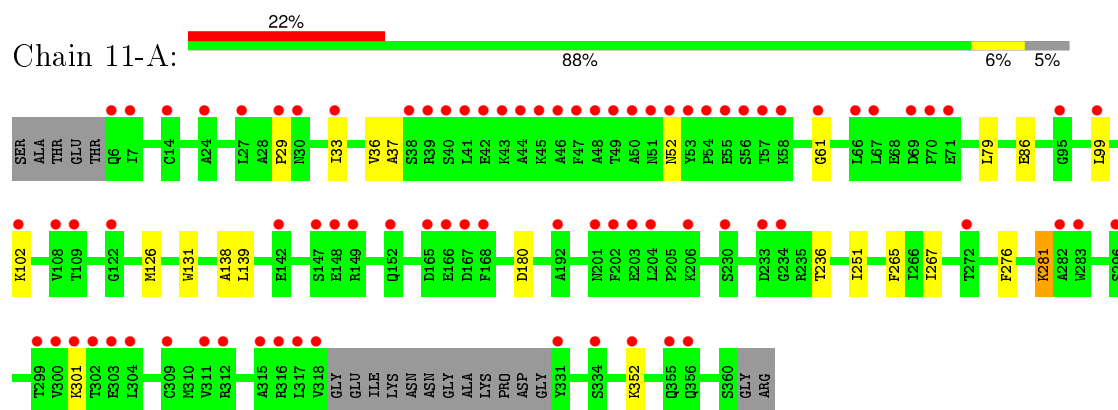
- Molecule 1: Probable oxidoreductase At4g09670



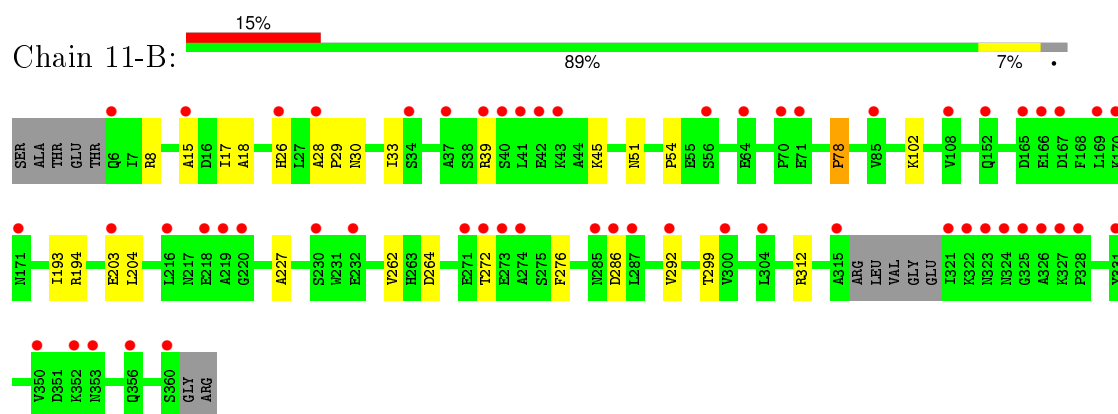
- Molecule 1: Probable oxidoreductase At4g09670



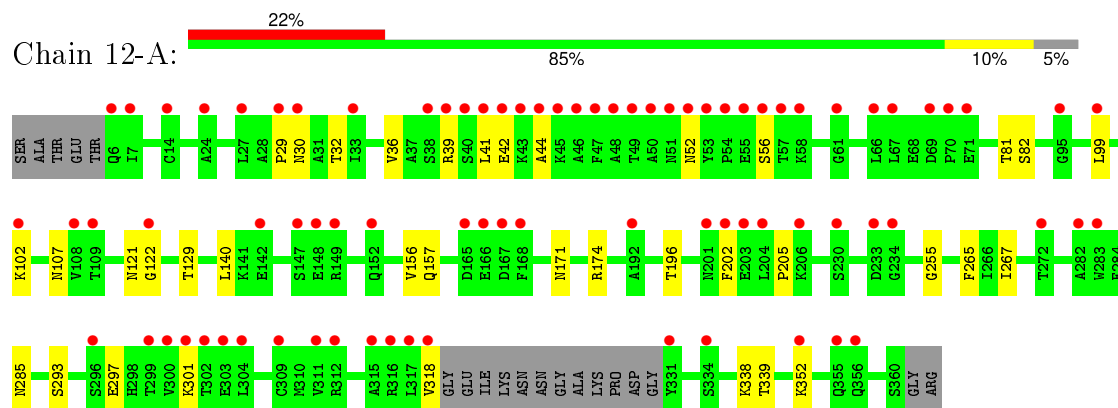
- Molecule 1: Probable oxidoreductase At4g09670



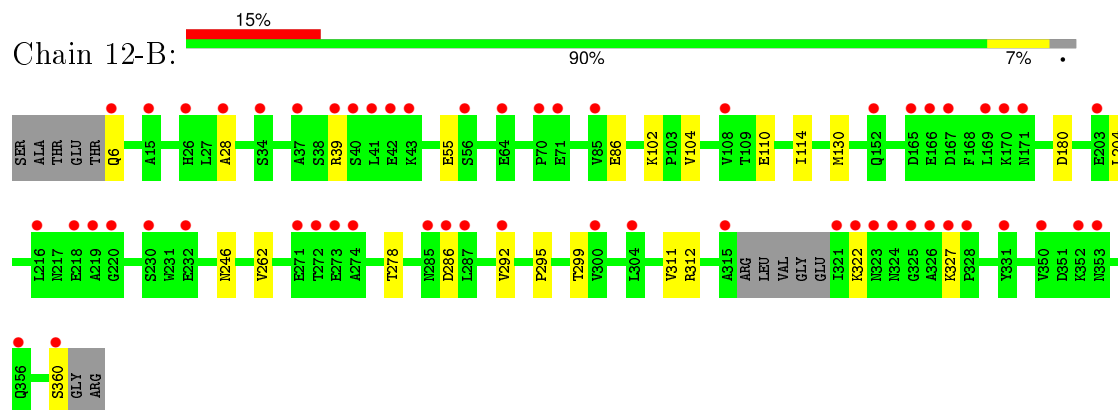
- Molecule 1: Probable oxidoreductase At4g09670



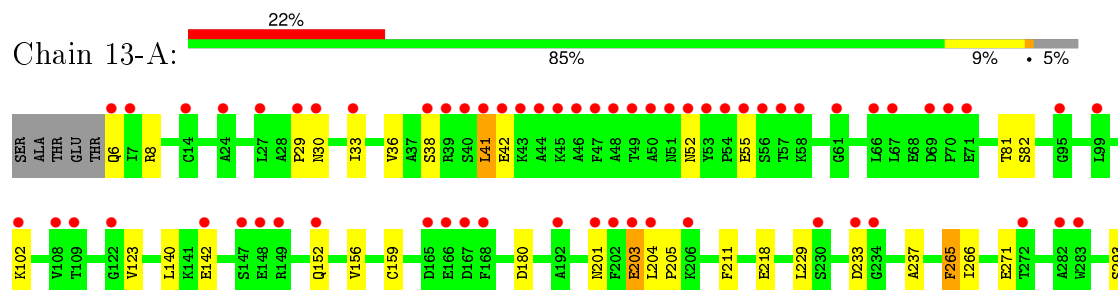
- Molecule 1: Probable oxidoreductase At4g09670

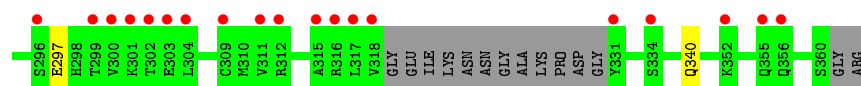


- Molecule 1: Probable oxidoreductase At4g09670

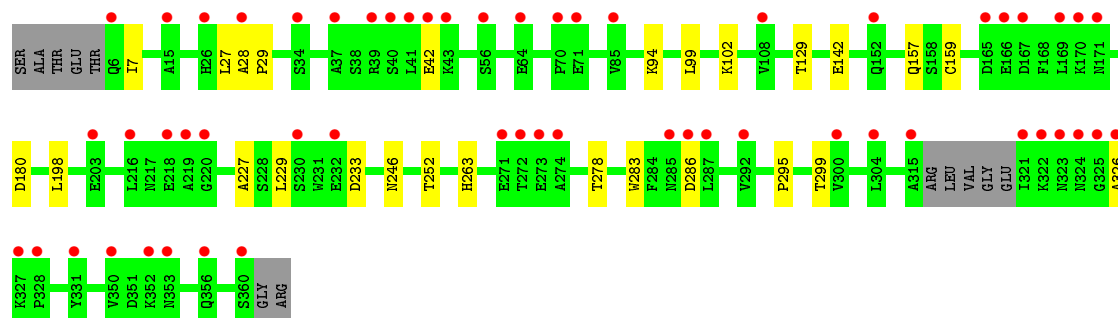


- Molecule 1: Probable oxidoreductase At4g09670

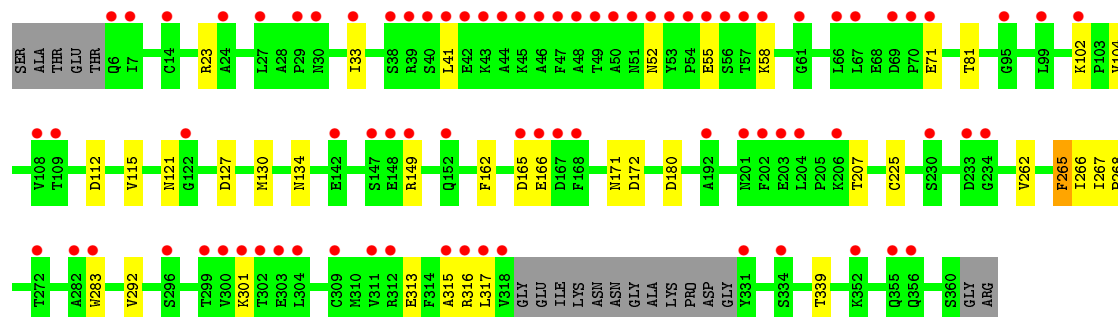
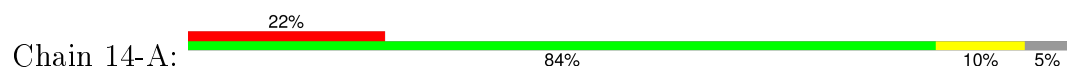




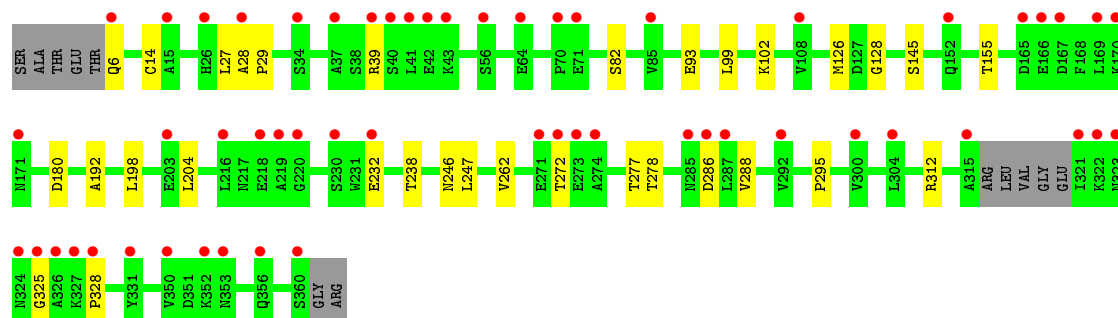
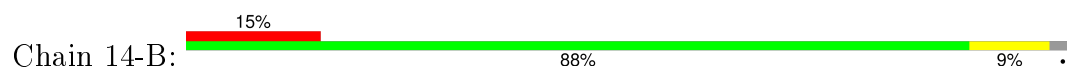
- Molecule 1: Probable oxidoreductase At4g09670



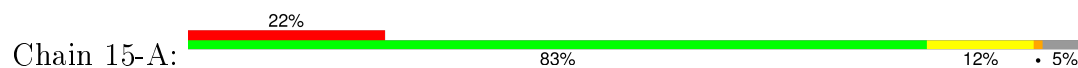
- Molecule 1: Probable oxidoreductase At4g09670

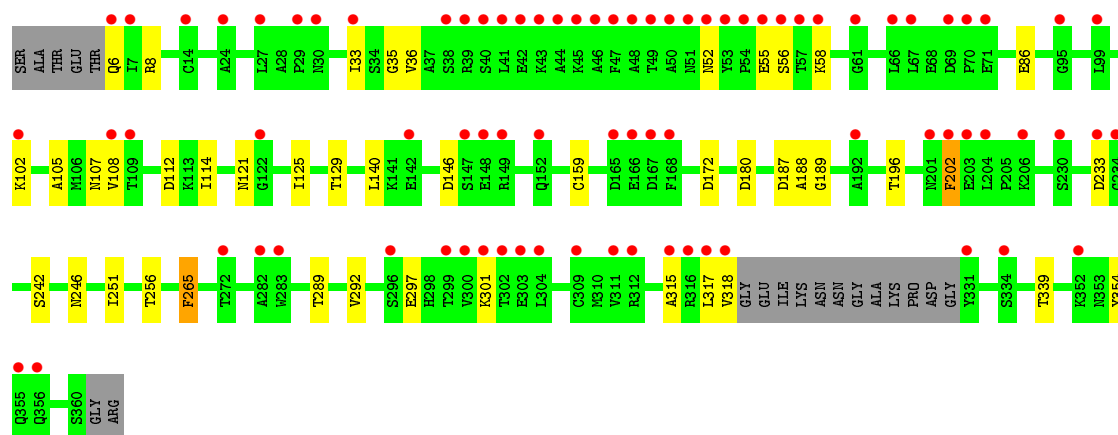


- Molecule 1: Probable oxidoreductase At4g09670

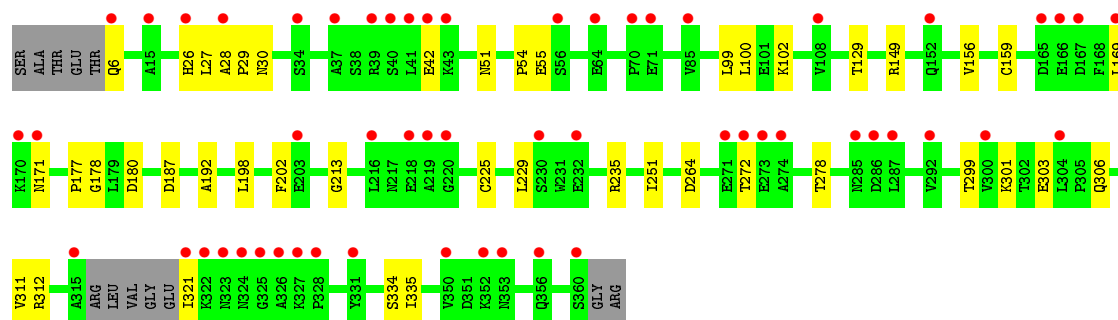
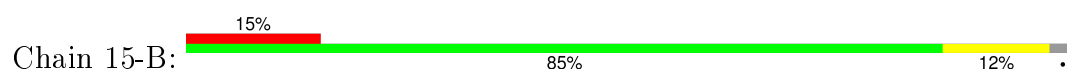


- Molecule 1: Probable oxidoreductase At4g09670

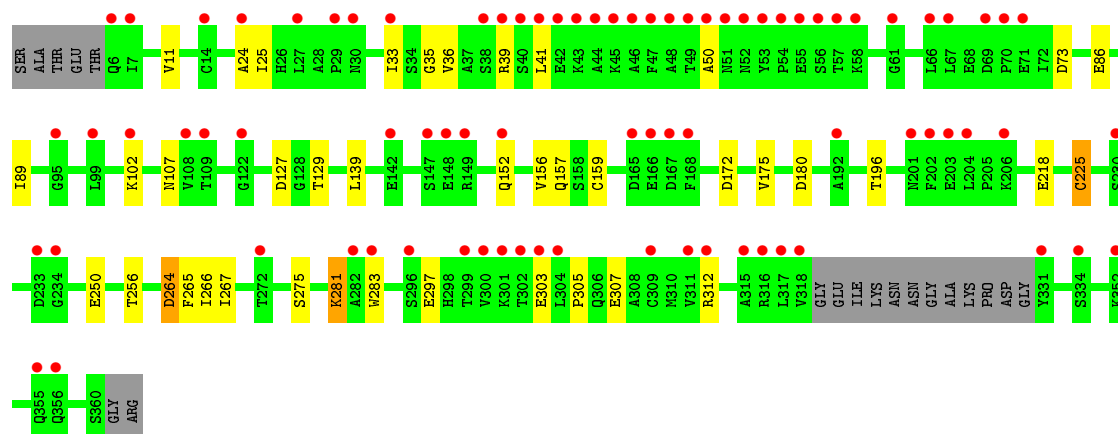
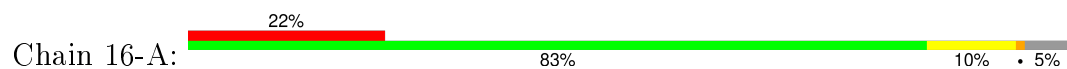




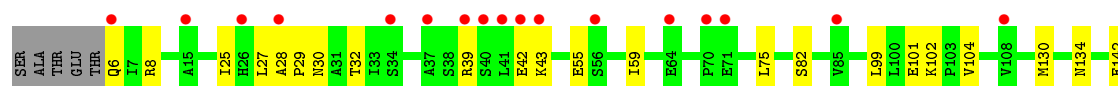
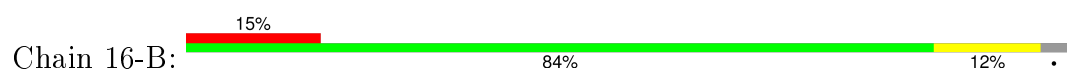
- Molecule 1: Probable oxidoreductase At4g09670

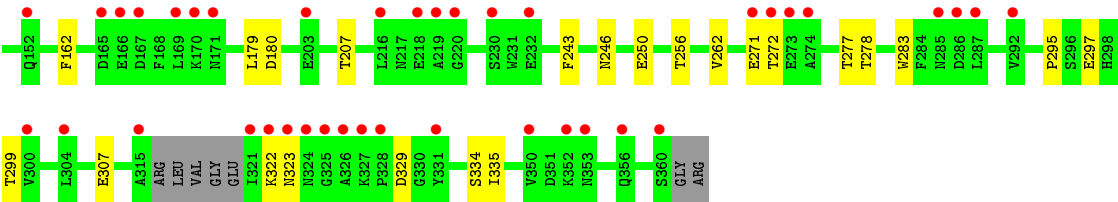


- Molecule 1: Probable oxidoreductase At4g09670



- Molecule 1: Probable oxidoreductase At4g09670





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.20Å 107.66Å 129.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.73 – 2.49 29.73 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.73-2.49) 98.4 (29.73-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.285 0.234 , 0.299	Depositor DCC
R_{free} test set	1472 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 92.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 28862 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	87408	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

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	1-A	0.34	0/2698	0.59	0/3656
1	1-B	0.35	0/2743	0.60	1/3716 (0.0%)
1	2-A	0.33	0/2698	0.57	0/3656
1	2-B	0.35	0/2743	0.60	0/3716
1	3-A	0.33	0/2698	0.59	0/3656
1	3-B	0.34	0/2743	0.58	0/3716
1	4-A	0.34	0/2698	0.59	0/3656
1	4-B	0.34	0/2743	0.60	0/3716
1	5-A	0.34	0/2698	0.59	0/3656
1	5-B	0.34	0/2743	0.58	0/3716
1	6-A	0.34	0/2698	0.59	0/3656
1	6-B	0.35	0/2743	0.60	1/3716 (0.0%)
1	7-A	0.33	0/2698	0.56	0/3656
1	7-B	0.34	0/2743	0.59	0/3716
1	8-A	0.34	0/2698	0.59	0/3656
1	8-B	0.35	0/2743	0.60	0/3716
1	9-A	0.33	0/2698	0.59	0/3656
1	9-B	0.35	0/2743	0.60	0/3716
1	10-A	0.34	0/2698	0.58	0/3656
1	10-B	0.35	0/2743	0.59	0/3716
1	11-A	0.34	0/2698	0.58	0/3656
1	11-B	0.35	0/2743	0.60	0/3716
1	12-A	0.34	0/2698	0.58	0/3656
1	12-B	0.34	0/2743	0.59	0/3716
1	13-A	0.36	0/2698	0.62	0/3656
1	13-B	0.37	0/2743	0.65	1/3716 (0.0%)
1	14-A	0.36	0/2698	0.62	0/3656
1	14-B	0.38	0/2743	0.64	1/3716 (0.0%)
1	15-A	0.37	0/2698	0.63	0/3656
1	15-B	0.38	0/2743	0.66	1/3716 (0.0%)
1	16-A	0.37	0/2698	0.62	0/3656
1	16-B	0.38	0/2743	0.63	1/3716 (0.0%)
All	All	0.35	0/87056	0.60	6/117952 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	15-B	27	LEU	N-CA-C	-6.95	92.23	111.00
1	16-B	27	LEU	N-CA-C	-6.42	93.67	111.00
1	13-B	27	LEU	N-CA-C	-5.91	95.04	111.00
1	14-B	27	LEU	N-CA-C	-5.71	95.58	111.00
1	6-B	27	LEU	N-CA-C	-5.42	96.37	111.00
1	1-B	234	GLY	N-CA-C	-5.29	99.86	113.10

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	1-A	2648	0	2642	0	0
1	1-B	2692	0	2680	0	0
1	2-A	2648	0	2642	0	0
1	2-B	2692	0	2680	0	0
1	3-A	2648	0	2642	0	0
1	3-B	2692	0	2680	0	0
1	4-A	2648	0	2642	0	0
1	4-B	2692	0	2680	0	0
1	5-A	2648	0	2642	0	0
1	5-B	2692	0	2680	0	0
1	6-A	2648	0	2642	0	0
1	6-B	2692	0	2680	0	0
1	7-A	2648	0	2642	0	0
1	7-B	2692	0	2680	0	0
1	8-A	2648	0	2642	0	0
1	8-B	2692	0	2680	0	0
1	9-A	2648	0	2642	0	0
1	9-B	2692	0	2680	0	0
1	10-A	2648	0	2642	0	0
1	10-B	2692	0	2680	0	0
1	11-A	2648	0	2642	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	11-B	2692	0	2680	0	0
1	12-A	2648	0	2642	0	0
1	12-B	2692	0	2680	0	0
1	13-A	2648	0	2642	0	0
1	13-B	2692	0	2680	0	0
1	14-A	2648	0	2642	0	0
1	14-B	2692	0	2680	0	0
1	15-A	2648	0	2642	0	0
1	15-B	2692	0	2680	0	0
1	16-A	2648	0	2642	0	0
1	16-B	2692	0	2680	0	0
2	1-A	60	0	0	0	0
2	1-B	63	0	0	0	0
2	2-A	58	0	0	0	0
2	2-B	65	0	0	0	0
2	3-A	62	0	0	0	0
2	3-B	61	0	0	0	0
2	4-A	60	0	0	0	0
2	4-B	63	0	0	0	0
2	5-A	59	0	0	0	0
2	5-B	64	0	0	0	0
2	6-A	60	0	0	0	0
2	6-B	63	0	0	0	0
2	7-A	61	0	0	0	0
2	7-B	62	0	0	0	0
2	8-A	56	0	0	0	0
2	8-B	67	0	0	0	0
2	9-A	60	0	0	0	0
2	9-B	63	0	0	0	0
2	10-A	59	0	0	0	0
2	10-B	64	0	0	0	0
2	11-A	60	0	0	0	0
2	11-B	63	0	0	0	0
2	12-A	61	0	0	0	0
2	12-B	62	0	0	0	0
2	13-A	62	0	0	0	0
2	13-B	61	0	0	0	0
2	14-A	59	0	0	0	0
2	14-B	64	0	0	0	0
2	15-A	59	0	0	0	0
2	15-B	64	0	0	0	0
2	16-A	60	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	16-B	63	0	0	0	0
All	All	87408	0	85152	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

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](#)

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	1-A	339/362 (94%)	294 (87%)	37 (11%)	8 (2%)	7	11
1	1-B	346/362 (96%)	300 (87%)	36 (10%)	10 (3%)	6	8
1	2-A	339/362 (94%)	300 (88%)	34 (10%)	5 (2%)	13	22
1	2-B	346/362 (96%)	307 (89%)	32 (9%)	7 (2%)	9	15
1	3-A	339/362 (94%)	276 (81%)	49 (14%)	14 (4%)	3	4
1	3-B	346/362 (96%)	286 (83%)	52 (15%)	8 (2%)	8	12
1	4-A	339/362 (94%)	287 (85%)	37 (11%)	15 (4%)	3	3
1	4-B	346/362 (96%)	315 (91%)	26 (8%)	5 (1%)	14	24
1	5-A	339/362 (94%)	295 (87%)	37 (11%)	7 (2%)	9	14
1	5-B	346/362 (96%)	298 (86%)	37 (11%)	11 (3%)	5	6
1	6-A	339/362 (94%)	298 (88%)	35 (10%)	6 (2%)	11	18
1	6-B	346/362 (96%)	309 (89%)	29 (8%)	8 (2%)	8	12
1	7-A	339/362 (94%)	291 (86%)	37 (11%)	11 (3%)	5	6
1	7-B	346/362 (96%)	294 (85%)	40 (12%)	12 (4%)	4	6
1	8-A	339/362 (94%)	280 (83%)	48 (14%)	11 (3%)	5	6
1	8-B	346/362 (96%)	303 (88%)	37 (11%)	6 (2%)	11	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	9-A	339/362 (94%)	299 (88%)	37 (11%)	3 (1%)	21	37
1	9-B	346/362 (96%)	309 (89%)	32 (9%)	5 (1%)	14	24
1	10-A	339/362 (94%)	294 (87%)	37 (11%)	8 (2%)	7	11
1	10-B	346/362 (96%)	296 (86%)	40 (12%)	10 (3%)	6	8
1	11-A	339/362 (94%)	284 (84%)	44 (13%)	11 (3%)	5	6
1	11-B	346/362 (96%)	288 (83%)	43 (12%)	15 (4%)	3	4
1	12-A	339/362 (94%)	272 (80%)	49 (14%)	18 (5%)	2	2
1	12-B	346/362 (96%)	294 (85%)	46 (13%)	6 (2%)	11	19
1	13-A	339/362 (94%)	281 (83%)	43 (13%)	15 (4%)	3	3
1	13-B	346/362 (96%)	309 (89%)	27 (8%)	10 (3%)	6	8
1	14-A	339/362 (94%)	288 (85%)	36 (11%)	15 (4%)	3	3
1	14-B	346/362 (96%)	302 (87%)	33 (10%)	11 (3%)	5	6
1	15-A	339/362 (94%)	265 (78%)	53 (16%)	21 (6%)	2	1
1	15-B	346/362 (96%)	282 (82%)	48 (14%)	16 (5%)	3	3
1	16-A	339/362 (94%)	270 (80%)	50 (15%)	19 (6%)	2	2
1	16-B	346/362 (96%)	291 (84%)	42 (12%)	13 (4%)	4	5
All	All	10960/11584 (95%)	9357 (85%)	1263 (12%)	340 (3%)	5	7

All (340) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	140	LEU
1	1-A	317	LEU
1	1-B	28	ALA
1	1-B	179	LEU
1	1-B	246	ASN
1	2-B	28	ALA
1	2-B	104	VAL
1	3-A	81	THR
1	3-A	172	ASP
1	3-A	233	ASP
1	3-A	317	LEU
1	3-B	235	ARG
1	3-B	276	PHE
1	4-A	200	ASN
1	4-A	233	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-B	28	ALA
1	4-B	247	LEU
1	5-A	233	ASP
1	5-A	303	GLU
1	5-B	24	ALA
1	5-B	25	ILE
1	5-B	27	LEU
1	5-B	246	ASN
1	6-B	30	ASN
1	7-B	30	ASN
1	7-B	286	ASP
1	8-A	54	PRO
1	8-A	265	PHE
1	8-B	28	ALA
1	8-B	179	LEU
1	10-B	28	ALA
1	10-B	295	PRO
1	11-A	138	ALA
1	11-B	30	ASN
1	11-B	203	GLU
1	12-A	140	LEU
1	12-A	285	ASN
1	12-B	28	ALA
1	12-B	104	VAL
1	13-A	204	LEU
1	13-A	233	ASP
1	13-A	265	PHE
1	13-A	293	SER
1	13-B	7	ILE
1	13-B	28	ALA
1	13-B	263	HIS
1	13-B	286	ASP
1	13-B	326	ALA
1	14-A	104	VAL
1	14-B	28	ALA
1	14-B	246	ASN
1	15-A	52	ASN
1	15-A	56	SER
1	15-A	233	ASP
1	15-A	354	TYR
1	15-B	28	ALA
1	15-B	30	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	15-B	202	PHE
1	15-B	303	GLU
1	15-B	334	SER
1	16-A	265	PHE
1	16-A	266	ILE
1	16-A	267	ILE
1	16-B	28	ALA
1	16-B	30	ASN
1	16-B	104	VAL
1	16-B	246	ASN
1	16-B	323	ASN
1	1-A	265	PHE
1	1-A	354	TYR
1	2-A	265	PHE
1	2-B	107	ASN
1	2-B	295	PRO
1	3-B	28	ALA
1	3-B	268	PRO
1	4-A	315	ALA
1	4-B	325	GLY
1	5-A	82	SER
1	5-A	281	LYS
1	5-A	316	ARG
1	5-B	286	ASP
1	6-A	140	LEU
1	6-A	265	PHE
1	6-B	128	GLY
1	6-B	246	ASN
1	6-B	295	PRO
1	7-A	162	PHE
1	7-A	281	LYS
1	7-B	179	LEU
1	7-B	246	ASN
1	7-B	295	PRO
1	8-A	17	ILE
1	8-A	52	ASN
1	8-A	317	LEU
1	9-A	265	PHE
1	10-A	265	PHE
1	10-A	317	LEU
1	10-B	174	ARG
1	10-B	179	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-B	246	ASN
1	11-A	131	TRP
1	11-A	251	ILE
1	11-B	15	ALA
1	11-B	18	ALA
1	11-B	194	ARG
1	11-B	264	ASP
1	11-B	276	PHE
1	11-B	286	ASP
1	12-A	52	ASN
1	12-A	82	SER
1	12-B	246	ASN
1	12-B	286	ASP
1	12-B	295	PRO
1	13-A	41	LEU
1	13-A	82	SER
1	13-B	129	THR
1	13-B	227	ALA
1	13-B	246	ASN
1	14-A	166	GLU
1	14-A	265	PHE
1	14-A	316	ARG
1	14-B	128	GLY
1	14-B	192	ALA
1	14-B	247	LEU
1	14-B	286	ASP
1	14-B	325	GLY
1	15-A	114	ILE
1	15-A	265	PHE
1	15-B	129	THR
1	15-B	178	GLY
1	15-B	192	ALA
1	15-B	235	ARG
1	15-B	264	ASP
1	15-B	299	THR
1	16-A	225	CYS
1	16-A	281	LYS
1	16-B	250	GLU
1	16-B	295	PRO
1	16-B	334	SER
1	1-A	232	GLU
1	1-A	315	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-B	352	LYS
1	2-A	140	LEU
1	2-A	171	ASN
1	2-B	82	SER
1	2-B	156	VAL
1	3-A	40	SER
1	3-A	281	LYS
1	3-A	295	PRO
1	4-A	30	ASN
1	4-A	82	SER
1	4-A	129	THR
1	4-A	165	ASP
1	4-A	281	LYS
1	4-A	282	ALA
1	4-A	317	LEU
1	5-A	129	THR
1	5-B	31	ALA
1	7-A	163	ALA
1	7-B	54	PRO
1	7-B	124	GLN
1	7-B	288	VAL
1	8-B	295	PRO
1	9-A	140	LEU
1	9-B	28	ALA
1	9-B	227	ALA
1	9-B	250	GLU
1	9-B	286	ASP
1	10-A	246	ASN
1	10-B	250	GLU
1	10-B	286	ASP
1	11-A	37	ALA
1	11-A	52	ASN
1	11-B	78	PRO
1	11-B	227	ALA
1	12-A	30	ASN
1	12-A	44	ALA
1	12-A	56	SER
1	12-A	129	THR
1	12-A	293	SER
1	13-A	30	ASN
1	13-A	38	SER
1	13-A	81	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	14-A	171	ASN
1	14-A	266	ILE
1	14-A	315	ALA
1	14-A	317	LEU
1	14-B	82	SER
1	14-B	295	PRO
1	15-A	105	ALA
1	15-A	121	ASN
1	15-A	129	THR
1	15-A	187	ASP
1	15-A	188	ALA
1	15-A	202	PHE
1	15-A	246	ASN
1	15-B	54	PRO
1	15-B	177	PRO
1	16-A	24	ALA
1	16-A	127	ASP
1	16-A	218	GLU
1	16-A	305	PRO
1	16-A	307	GLU
1	1-B	192	ALA
1	1-B	286	ASP
1	2-B	54	PRO
1	3-A	105	ALA
1	3-A	121	ASN
1	3-A	137	THR
1	3-A	267	ILE
1	3-A	315	ALA
1	3-B	54	PRO
1	4-A	81	THR
1	4-A	267	ILE
1	4-A	286	ASP
1	4-B	293	SER
1	5-B	213	GLY
1	5-B	283	TRP
1	6-A	316	ARG
1	6-B	79	LEU
1	7-A	131	TRP
1	7-A	290	ALA
1	7-A	316	ARG
1	7-B	352	LYS
1	8-A	36	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-A	140	LEU
1	8-A	267	ILE
1	8-A	315	ALA
1	8-B	131	TRP
1	11-B	29	PRO
1	12-A	29	PRO
1	12-A	32	THR
1	12-A	107	ASN
1	12-A	205	PRO
1	13-A	29	PRO
1	13-A	52	ASN
1	13-A	203	GLU
1	13-A	266	ILE
1	13-B	94	LYS
1	14-A	52	ASN
1	14-A	81	THR
1	14-A	149	ARG
1	14-A	267	ILE
1	14-B	328	PRO
1	15-A	86	GLU
1	15-A	189	GLY
1	15-A	242	SER
1	15-A	315	ALA
1	15-B	306	GLN
1	16-A	107	ASN
1	16-A	250	GLU
1	16-B	82	SER
1	1-A	160	PHE
1	1-A	267	ILE
1	1-B	156	VAL
1	1-B	295	PRO
1	2-A	267	ILE
1	2-A	316	ARG
1	3-A	36	VAL
1	3-B	246	ASN
1	5-A	267	ILE
1	5-B	288	VAL
1	5-B	295	PRO
1	6-A	267	ILE
1	6-A	317	LEU
1	7-A	29	PRO
1	7-A	79	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-A	267	ILE
1	7-B	283	TRP
1	8-A	214	ALA
1	8-B	58	LYS
1	9-A	267	ILE
1	9-B	54	PRO
1	10-A	267	ILE
1	10-A	315	ALA
1	10-B	120	ALA
1	10-B	233	ASP
1	10-B	322	LYS
1	11-A	79	LEU
1	11-A	267	ILE
1	11-B	28	ALA
1	11-B	54	PRO
1	11-B	193	ILE
1	12-A	81	THR
1	12-B	114	ILE
1	13-A	205	PRO
1	13-A	237	ALA
1	14-A	225	CYS
1	15-A	317	LEU
1	16-A	35	GLY
1	16-A	50	ALA
1	16-A	129	THR
1	16-A	175	VAL
1	16-A	264	ASP
1	16-B	59	ILE
1	16-B	179	LEU
1	3-A	79	LEU
1	6-A	299	THR
1	7-A	160	PHE
1	7-A	317	LEU
1	8-B	288	VAL
1	11-A	281	LYS
1	12-A	122	GLY
1	15-A	292	VAL
1	15-B	213	GLY
1	10-A	11	VAL
1	10-A	215	VAL
1	11-A	36	VAL
1	12-A	36	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	12-A	267	ILE
1	16-B	25	ILE
1	4-A	268	PRO
1	4-B	54	PRO
1	6-B	122	GLY
1	7-B	122	GLY
1	11-B	204	LEU
1	12-A	255	GLY
1	14-B	288	VAL
1	15-A	35	GLY
1	15-A	125	ILE
1	1-B	234	GLY
1	1-B	357	ILE
1	6-B	123	VAL
1	6-B	288	VAL
1	7-B	175	VAL
1	10-A	36	VAL
1	13-B	295	PRO
1	16-A	11	VAL
1	3-B	78	PRO
1	3-B	288	VAL
1	4-A	29	PRO
1	11-A	61	GLY
1	14-A	115	VAL
1	16-A	25	ILE
1	5-B	78	PRO
1	8-A	350	VAL
1	11-A	29	PRO
1	14-A	268	PRO
1	15-B	29	PRO
1	16-B	29	PRO

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	286/293 (98%)	266 (93%)	20 (7%)	19	34
1	1-B	290/293 (99%)	276 (95%)	14 (5%)	31	55
1	2-A	286/293 (98%)	269 (94%)	17 (6%)	24	44
1	2-B	290/293 (99%)	280 (97%)	10 (3%)	44	72
1	3-A	286/293 (98%)	263 (92%)	23 (8%)	15	28
1	3-B	290/293 (99%)	275 (95%)	15 (5%)	29	51
1	4-A	286/293 (98%)	267 (93%)	19 (7%)	21	38
1	4-B	290/293 (99%)	280 (97%)	10 (3%)	44	72
1	5-A	286/293 (98%)	268 (94%)	18 (6%)	22	40
1	5-B	290/293 (99%)	278 (96%)	12 (4%)	37	63
1	6-A	286/293 (98%)	270 (94%)	16 (6%)	26	47
1	6-B	290/293 (99%)	277 (96%)	13 (4%)	34	59
1	7-A	286/293 (98%)	264 (92%)	22 (8%)	16	30
1	7-B	290/293 (99%)	276 (95%)	14 (5%)	31	55
1	8-A	286/293 (98%)	273 (96%)	13 (4%)	34	59
1	8-B	290/293 (99%)	272 (94%)	18 (6%)	23	41
1	9-A	286/293 (98%)	265 (93%)	21 (7%)	17	32
1	9-B	290/293 (99%)	276 (95%)	14 (5%)	31	55
1	10-A	286/293 (98%)	268 (94%)	18 (6%)	22	40
1	10-B	290/293 (99%)	279 (96%)	11 (4%)	40	67
1	11-A	286/293 (98%)	273 (96%)	13 (4%)	34	59
1	11-B	290/293 (99%)	276 (95%)	14 (5%)	31	55
1	12-A	286/293 (98%)	267 (93%)	19 (7%)	21	38
1	12-B	290/293 (99%)	272 (94%)	18 (6%)	23	41
1	13-A	286/293 (98%)	262 (92%)	24 (8%)	14	25
1	13-B	290/293 (99%)	275 (95%)	15 (5%)	29	51
1	14-A	286/293 (98%)	262 (92%)	24 (8%)	14	25
1	14-B	290/293 (99%)	270 (93%)	20 (7%)	19	35
1	15-A	286/293 (98%)	261 (91%)	25 (9%)	13	24
1	15-B	290/293 (99%)	264 (91%)	26 (9%)	12	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	16-A	286/293 (98%)	261 (91%)	25 (9%)	13	24
1	16-B	290/293 (99%)	259 (89%)	31 (11%)	8	15
All	All	9216/9376 (98%)	8644 (94%)	572 (6%)	23	41

All (572) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	6	GLN
1	1-A	23	ARG
1	1-A	33	ILE
1	1-A	55	GLU
1	1-A	99	LEU
1	1-A	102	LYS
1	1-A	130	MSE
1	1-A	139	LEU
1	1-A	180	ASP
1	1-A	196	THR
1	1-A	201	ASN
1	1-A	211	PHE
1	1-A	229	LEU
1	1-A	250	GLU
1	1-A	256	THR
1	1-A	264	ASP
1	1-A	265	PHE
1	1-A	289	THR
1	1-A	339	THR
1	1-A	352	LYS
1	1-B	42	GLU
1	1-B	71	GLU
1	1-B	102	LYS
1	1-B	142	GLU
1	1-B	180	ASP
1	1-B	204	LEU
1	1-B	232	GLU
1	1-B	243	PHE
1	1-B	244	LEU
1	1-B	262	VAL
1	1-B	272	THR
1	1-B	292	VAL
1	1-B	312	ARG
1	1-B	354	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-A	33	ILE
1	2-A	41	LEU
1	2-A	55	GLU
1	2-A	99	LEU
1	2-A	102	LYS
1	2-A	130	MSE
1	2-A	180	ASP
1	2-A	196	THR
1	2-A	201	ASN
1	2-A	216	LEU
1	2-A	218	GLU
1	2-A	254	ILE
1	2-A	256	THR
1	2-A	264	ASP
1	2-A	265	PHE
1	2-A	297	GLU
1	2-A	352	LYS
1	2-B	6	GLN
1	2-B	43	LYS
1	2-B	51	ASN
1	2-B	55	GLU
1	2-B	101	GLU
1	2-B	102	LYS
1	2-B	112	ASP
1	2-B	272	THR
1	2-B	292	VAL
1	2-B	299	THR
1	3-A	22	SER
1	3-A	23	ARG
1	3-A	39	ARG
1	3-A	68	GLU
1	3-A	101	GLU
1	3-A	102	LYS
1	3-A	113	LYS
1	3-A	116	ASP
1	3-A	124	GLN
1	3-A	130	MSE
1	3-A	146	ASP
1	3-A	165	ASP
1	3-A	169	LEU
1	3-A	172	ASP
1	3-A	232	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	3-A	257	LYS
1	3-A	276	PHE
1	3-A	281	LYS
1	3-A	283	TRP
1	3-A	297	GLU
1	3-A	317	LEU
1	3-A	343	VAL
1	3-A	352	LYS
1	3-B	39	ARG
1	3-B	53	TYR
1	3-B	55	GLU
1	3-B	73	ASP
1	3-B	75	LEU
1	3-B	101	GLU
1	3-B	102	LYS
1	3-B	124	GLN
1	3-B	159	CYS
1	3-B	187	ASP
1	3-B	198	LEU
1	3-B	204	LEU
1	3-B	229	LEU
1	3-B	273	GLU
1	3-B	311	VAL
1	4-A	6	GLN
1	4-A	32	THR
1	4-A	33	ILE
1	4-A	39	ARG
1	4-A	41	LEU
1	4-A	55	GLU
1	4-A	99	LEU
1	4-A	102	LYS
1	4-A	139	LEU
1	4-A	146	ASP
1	4-A	159	CYS
1	4-A	180	ASP
1	4-A	200	ASN
1	4-A	201	ASN
1	4-A	259	THR
1	4-A	265	PHE
1	4-A	278	THR
1	4-A	283	TRP
1	4-A	344	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-B	55	GLU
1	4-B	102	LYS
1	4-B	180	ASP
1	4-B	198	LEU
1	4-B	204	LEU
1	4-B	233	ASP
1	4-B	299	THR
1	4-B	311	VAL
1	4-B	312	ARG
1	4-B	339	THR
1	5-A	23	ARG
1	5-A	33	ILE
1	5-A	39	ARG
1	5-A	42	GLU
1	5-A	55	GLU
1	5-A	89	ILE
1	5-A	99	LEU
1	5-A	102	LYS
1	5-A	123	VAL
1	5-A	139	LEU
1	5-A	148	GLU
1	5-A	161	SER
1	5-A	180	ASP
1	5-A	265	PHE
1	5-A	283	TRP
1	5-A	284	PHE
1	5-A	287	LEU
1	5-A	339	THR
1	5-B	78	PRO
1	5-B	101	GLU
1	5-B	170	LYS
1	5-B	180	ASP
1	5-B	233	ASP
1	5-B	238	THR
1	5-B	262	VAL
1	5-B	272	THR
1	5-B	284	PHE
1	5-B	292	VAL
1	5-B	299	THR
1	5-B	312	ARG
1	6-A	6	GLN
1	6-A	33	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-A	55	GLU
1	6-A	99	LEU
1	6-A	102	LYS
1	6-A	140	LEU
1	6-A	146	ASP
1	6-A	180	ASP
1	6-A	200	ASN
1	6-A	264	ASP
1	6-A	265	PHE
1	6-A	281	LYS
1	6-A	297	GLU
1	6-A	318	VAL
1	6-A	334	SER
1	6-A	339	THR
1	6-B	39	ARG
1	6-B	102	LYS
1	6-B	108	VAL
1	6-B	158	SER
1	6-B	180	ASP
1	6-B	232	GLU
1	6-B	262	VAL
1	6-B	272	THR
1	6-B	278	THR
1	6-B	283	TRP
1	6-B	299	THR
1	6-B	312	ARG
1	6-B	339	THR
1	7-A	33	ILE
1	7-A	41	LEU
1	7-A	55	GLU
1	7-A	68	GLU
1	7-A	86	GLU
1	7-A	99	LEU
1	7-A	101	GLU
1	7-A	102	LYS
1	7-A	108	VAL
1	7-A	123	VAL
1	7-A	126	MSE
1	7-A	139	LEU
1	7-A	142	GLU
1	7-A	162	PHE
1	7-A	180	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	7-A	201	ASN
1	7-A	249	MSE
1	7-A	256	THR
1	7-A	283	TRP
1	7-A	318	VAL
1	7-A	339	THR
1	7-A	344	ASP
1	7-B	27	LEU
1	7-B	30	ASN
1	7-B	32	THR
1	7-B	42	GLU
1	7-B	55	GLU
1	7-B	102	LYS
1	7-B	112	ASP
1	7-B	174	ARG
1	7-B	180	ASP
1	7-B	207	THR
1	7-B	272	THR
1	7-B	283	TRP
1	7-B	284	PHE
1	7-B	312	ARG
1	8-A	33	ILE
1	8-A	75	LEU
1	8-A	99	LEU
1	8-A	102	LYS
1	8-A	123	VAL
1	8-A	180	ASP
1	8-A	201	ASN
1	8-A	207	THR
1	8-A	256	THR
1	8-A	265	PHE
1	8-A	297	GLU
1	8-A	301	LYS
1	8-A	339	THR
1	8-B	51	ASN
1	8-B	58	LYS
1	8-B	99	LEU
1	8-B	101	GLU
1	8-B	102	LYS
1	8-B	107	ASN
1	8-B	112	ASP
1	8-B	180	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-B	217	ASN
1	8-B	233	ASP
1	8-B	250	GLU
1	8-B	272	THR
1	8-B	278	THR
1	8-B	283	TRP
1	8-B	292	VAL
1	8-B	299	THR
1	8-B	311	VAL
1	8-B	312	ARG
1	9-A	33	ILE
1	9-A	39	ARG
1	9-A	42	GLU
1	9-A	55	GLU
1	9-A	58	LYS
1	9-A	99	LEU
1	9-A	102	LYS
1	9-A	108	VAL
1	9-A	126	MSE
1	9-A	130	MSE
1	9-A	134	ASN
1	9-A	139	LEU
1	9-A	180	ASP
1	9-A	201	ASN
1	9-A	256	THR
1	9-A	264	ASP
1	9-A	265	PHE
1	9-A	297	GLU
1	9-A	317	LEU
1	9-A	318	VAL
1	9-A	339	THR
1	9-B	27	LEU
1	9-B	42	GLU
1	9-B	55	GLU
1	9-B	99	LEU
1	9-B	102	LYS
1	9-B	130	MSE
1	9-B	154	LYS
1	9-B	180	ASP
1	9-B	198	LEU
1	9-B	238	THR
1	9-B	244	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-B	272	THR
1	9-B	312	ARG
1	9-B	339	THR
1	10-A	6	GLN
1	10-A	33	ILE
1	10-A	41	LEU
1	10-A	55	GLU
1	10-A	99	LEU
1	10-A	102	LYS
1	10-A	139	LEU
1	10-A	180	ASP
1	10-A	196	THR
1	10-A	201	ASN
1	10-A	218	GLU
1	10-A	264	ASP
1	10-A	265	PHE
1	10-A	297	GLU
1	10-A	301	LYS
1	10-A	339	THR
1	10-A	344	ASP
1	10-A	352	LYS
1	10-B	29	PRO
1	10-B	39	ARG
1	10-B	99	LEU
1	10-B	102	LYS
1	10-B	130	MSE
1	10-B	180	ASP
1	10-B	204	LEU
1	10-B	278	THR
1	10-B	292	VAL
1	10-B	299	THR
1	10-B	312	ARG
1	11-A	33	ILE
1	11-A	86	GLU
1	11-A	99	LEU
1	11-A	102	LYS
1	11-A	126	MSE
1	11-A	139	LEU
1	11-A	180	ASP
1	11-A	236	THR
1	11-A	265	PHE
1	11-A	276	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	11-A	281	LYS
1	11-A	301	LYS
1	11-A	352	LYS
1	11-B	8	ARG
1	11-B	17	ILE
1	11-B	26	HIS
1	11-B	33	ILE
1	11-B	39	ARG
1	11-B	45	LYS
1	11-B	51	ASN
1	11-B	78	PRO
1	11-B	102	LYS
1	11-B	262	VAL
1	11-B	272	THR
1	11-B	292	VAL
1	11-B	299	THR
1	11-B	312	ARG
1	12-A	39	ARG
1	12-A	41	LEU
1	12-A	42	GLU
1	12-A	99	LEU
1	12-A	102	LYS
1	12-A	121	ASN
1	12-A	156	VAL
1	12-A	157	GLN
1	12-A	171	ASN
1	12-A	174	ARG
1	12-A	196	THR
1	12-A	202	PHE
1	12-A	265	PHE
1	12-A	297	GLU
1	12-A	301	LYS
1	12-A	318	VAL
1	12-A	338	LYS
1	12-A	339	THR
1	12-A	352	LYS
1	12-B	6	GLN
1	12-B	39	ARG
1	12-B	55	GLU
1	12-B	86	GLU
1	12-B	102	LYS
1	12-B	110	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	12-B	130	MSE
1	12-B	180	ASP
1	12-B	204	LEU
1	12-B	262	VAL
1	12-B	278	THR
1	12-B	292	VAL
1	12-B	299	THR
1	12-B	311	VAL
1	12-B	312	ARG
1	12-B	322	LYS
1	12-B	327	LYS
1	12-B	360	SER
1	13-A	6	GLN
1	13-A	8	ARG
1	13-A	33	ILE
1	13-A	36	VAL
1	13-A	41	LEU
1	13-A	42	GLU
1	13-A	55	GLU
1	13-A	102	LYS
1	13-A	123	VAL
1	13-A	140	LEU
1	13-A	142	GLU
1	13-A	152	GLN
1	13-A	156	VAL
1	13-A	159	CYS
1	13-A	180	ASP
1	13-A	201	ASN
1	13-A	203	GLU
1	13-A	211	PHE
1	13-A	218	GLU
1	13-A	229	LEU
1	13-A	265	PHE
1	13-A	271	GLU
1	13-A	297	GLU
1	13-A	340	GLN
1	13-B	29	PRO
1	13-B	42	GLU
1	13-B	99	LEU
1	13-B	102	LYS
1	13-B	142	GLU
1	13-B	157	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13-B	159	CYS
1	13-B	180	ASP
1	13-B	198	LEU
1	13-B	229	LEU
1	13-B	233	ASP
1	13-B	252	THR
1	13-B	278	THR
1	13-B	283	TRP
1	13-B	299	THR
1	14-A	23	ARG
1	14-A	33	ILE
1	14-A	41	LEU
1	14-A	55	GLU
1	14-A	58	LYS
1	14-A	71	GLU
1	14-A	102	LYS
1	14-A	112	ASP
1	14-A	121	ASN
1	14-A	127	ASP
1	14-A	130	MSE
1	14-A	134	ASN
1	14-A	162	PHE
1	14-A	165	ASP
1	14-A	172	ASP
1	14-A	180	ASP
1	14-A	207	THR
1	14-A	262	VAL
1	14-A	265	PHE
1	14-A	283	TRP
1	14-A	292	VAL
1	14-A	301	LYS
1	14-A	313	GLU
1	14-A	339	THR
1	14-B	6	GLN
1	14-B	14	CYS
1	14-B	29	PRO
1	14-B	39	ARG
1	14-B	93	GLU
1	14-B	99	LEU
1	14-B	102	LYS
1	14-B	126	MSE
1	14-B	145	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	14-B	155	THR
1	14-B	180	ASP
1	14-B	198	LEU
1	14-B	204	LEU
1	14-B	232	GLU
1	14-B	238	THR
1	14-B	262	VAL
1	14-B	272	THR
1	14-B	277	THR
1	14-B	278	THR
1	14-B	312	ARG
1	15-A	6	GLN
1	15-A	8	ARG
1	15-A	33	ILE
1	15-A	36	VAL
1	15-A	55	GLU
1	15-A	58	LYS
1	15-A	102	LYS
1	15-A	107	ASN
1	15-A	108	VAL
1	15-A	112	ASP
1	15-A	140	LEU
1	15-A	146	ASP
1	15-A	159	CYS
1	15-A	172	ASP
1	15-A	180	ASP
1	15-A	196	THR
1	15-A	202	PHE
1	15-A	251	ILE
1	15-A	256	THR
1	15-A	265	PHE
1	15-A	289	THR
1	15-A	297	GLU
1	15-A	301	LYS
1	15-A	318	VAL
1	15-A	339	THR
1	15-B	6	GLN
1	15-B	26	HIS
1	15-B	42	GLU
1	15-B	51	ASN
1	15-B	55	GLU
1	15-B	99	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	15-B	100	LEU
1	15-B	102	LYS
1	15-B	149	ARG
1	15-B	156	VAL
1	15-B	159	CYS
1	15-B	169	LEU
1	15-B	171	ASN
1	15-B	180	ASP
1	15-B	187	ASP
1	15-B	198	LEU
1	15-B	225	CYS
1	15-B	229	LEU
1	15-B	251	ILE
1	15-B	272	THR
1	15-B	278	THR
1	15-B	301	LYS
1	15-B	311	VAL
1	15-B	312	ARG
1	15-B	321	ILE
1	15-B	335	ILE
1	16-A	33	ILE
1	16-A	36	VAL
1	16-A	39	ARG
1	16-A	41	LEU
1	16-A	73	ASP
1	16-A	86	GLU
1	16-A	89	ILE
1	16-A	102	LYS
1	16-A	139	LEU
1	16-A	152	GLN
1	16-A	156	VAL
1	16-A	157	GLN
1	16-A	159	CYS
1	16-A	172	ASP
1	16-A	180	ASP
1	16-A	196	THR
1	16-A	225	CYS
1	16-A	256	THR
1	16-A	264	ASP
1	16-A	275	SER
1	16-A	281	LYS
1	16-A	283	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16-A	297	GLU
1	16-A	303	GLU
1	16-A	312	ARG
1	16-B	6	GLN
1	16-B	8	ARG
1	16-B	32	THR
1	16-B	39	ARG
1	16-B	42	GLU
1	16-B	43	LYS
1	16-B	55	GLU
1	16-B	75	LEU
1	16-B	99	LEU
1	16-B	101	GLU
1	16-B	102	LYS
1	16-B	130	MSE
1	16-B	134	ASN
1	16-B	142	GLU
1	16-B	162	PHE
1	16-B	180	ASP
1	16-B	207	THR
1	16-B	243	PHE
1	16-B	256	THR
1	16-B	262	VAL
1	16-B	271	GLU
1	16-B	272	THR
1	16-B	277	THR
1	16-B	278	THR
1	16-B	283	TRP
1	16-B	297	GLU
1	16-B	299	THR
1	16-B	307	GLU
1	16-B	322	LYS
1	16-B	329	ASP
1	16-B	335	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	51	ASN
1	1-A	201	ASN
1	1-A	263	HIS
1	1-A	298	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-A	355	GLN
1	2-A	51	ASN
1	2-A	201	ASN
1	2-B	51	ASN
1	2-B	157	GLN
1	2-B	340	GLN
1	3-A	6	GLN
1	3-A	124	GLN
1	3-A	157	GLN
1	3-A	200	ASN
1	3-A	356	GLN
1	3-B	124	GLN
1	4-A	51	ASN
1	4-A	157	GLN
1	4-A	200	ASN
1	4-A	201	ASN
1	4-A	355	GLN
1	4-B	133	HIS
1	4-B	246	ASN
1	5-A	152	GLN
1	5-A	201	ASN
1	5-A	355	GLN
1	5-B	26	HIS
1	6-A	51	ASN
1	6-A	200	ASN
1	6-A	201	ASN
1	6-A	263	HIS
1	6-A	298	HIS
1	6-B	124	GLN
1	6-B	133	HIS
1	6-B	157	GLN
1	6-B	246	ASN
1	6-B	356	GLN
1	7-A	124	GLN
1	7-A	157	GLN
1	7-A	201	ASN
1	7-A	356	GLN
1	7-B	124	GLN
1	8-A	157	GLN
1	8-A	201	ASN
1	8-A	340	GLN
1	8-A	356	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	8-B	107	ASN
1	8-B	121	ASN
1	8-B	133	HIS
1	8-B	157	GLN
1	8-B	217	ASN
1	9-A	51	ASN
1	9-A	124	GLN
1	9-A	134	ASN
1	9-A	200	ASN
1	9-A	201	ASN
1	9-A	306	GLN
1	9-B	152	GLN
1	10-A	51	ASN
1	10-A	263	HIS
1	10-A	355	GLN
1	10-B	124	GLN
1	10-B	355	GLN
1	10-B	356	GLN
1	11-A	60	HIS
1	11-A	121	ASN
1	11-A	124	GLN
1	11-A	152	GLN
1	11-A	201	ASN
1	11-A	355	GLN
1	11-A	356	GLN
1	11-B	51	ASN
1	11-B	60	HIS
1	11-B	124	GLN
1	12-A	30	ASN
1	12-A	51	ASN
1	12-A	124	GLN
1	12-A	171	ASN
1	12-A	201	ASN
1	12-A	355	GLN
1	12-B	133	HIS
1	12-B	217	ASN
1	13-A	51	ASN
1	13-A	107	ASN
1	13-A	201	ASN
1	13-A	298	HIS
1	13-B	157	GLN
1	13-B	246	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	14-A	134	ASN
1	14-A	152	GLN
1	14-A	201	ASN
1	14-A	263	HIS
1	14-B	124	GLN
1	14-B	133	HIS
1	14-B	356	GLN
1	15-A	107	ASN
1	15-A	124	GLN
1	15-A	356	GLN
1	15-B	124	GLN
1	15-B	133	HIS
1	15-B	134	ASN
1	15-B	157	GLN
1	15-B	263	HIS
1	15-B	298	HIS
1	15-B	306	GLN
1	16-A	152	GLN
1	16-A	201	ASN
1	16-A	246	ASN
1	16-A	355	GLN
1	16-A	356	GLN
1	16-B	6	GLN
1	16-B	26	HIS
1	16-B	134	ASN
1	16-B	152	GLN
1	16-B	157	GLN
1	16-B	306	GLN

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, 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	1-A	337/362 (93%)	1.21	81 (24%) 1 1	15, 33, 53, 80	337 (100%)
1	1-B	344/362 (95%)	0.94	56 (16%) 2 2	16, 31, 46, 53	344 (100%)
1	2-A	337/362 (93%)	1.21	81 (24%) 1 1	15, 33, 53, 80	337 (100%)
1	2-B	344/362 (95%)	0.94	56 (16%) 2 2	16, 31, 46, 53	344 (100%)
1	3-A	337/362 (93%)	1.21	81 (24%) 1 1	15, 33, 53, 80	337 (100%)
1	3-B	344/362 (95%)	0.94	56 (16%) 2 2	16, 31, 46, 53	344 (100%)
1	4-A	337/362 (93%)	1.21	81 (24%) 1 1	15, 33, 53, 80	337 (100%)
1	4-B	344/362 (95%)	0.94	56 (16%) 2 2	16, 31, 46, 53	344 (100%)
1	5-A	337/362 (93%)	1.21	81 (24%) 1 1	15, 33, 53, 80	337 (100%)
1	5-B	344/362 (95%)	0.94	56 (16%) 2 2	16, 31, 46, 53	344 (100%)
1	6-A	337/362 (93%)	1.21	81 (24%) 1 1	15, 33, 53, 80	337 (100%)
1	6-B	344/362 (95%)	0.94	56 (16%) 2 2	16, 31, 46, 53	344 (100%)
1	7-A	337/362 (93%)	1.21	81 (24%) 1 1	15, 33, 53, 80	337 (100%)
1	7-B	344/362 (95%)	0.94	56 (16%) 2 2	16, 31, 46, 53	344 (100%)
1	8-A	337/362 (93%)	1.21	81 (24%) 1 1	15, 33, 53, 80	337 (100%)
1	8-B	344/362 (95%)	0.94	56 (16%) 2 2	16, 31, 46, 53	344 (100%)
1	9-A	337/362 (93%)	1.21	81 (24%) 1 1	15, 33, 53, 80	337 (100%)
1	9-B	344/362 (95%)	0.94	56 (16%) 2 2	16, 31, 46, 53	344 (100%)
1	10-A	337/362 (93%)	1.21	81 (24%) 1 1	15, 33, 53, 80	337 (100%)
1	10-B	344/362 (95%)	0.94	56 (16%) 2 2	16, 31, 46, 53	344 (100%)
1	11-A	337/362 (93%)	1.21	81 (24%) 1 1	15, 33, 53, 80	337 (100%)
1	11-B	344/362 (95%)	0.94	56 (16%) 2 2	16, 31, 46, 53	344 (100%)
1	12-A	337/362 (93%)	1.21	81 (24%) 1 1	15, 33, 53, 80	337 (100%)
1	12-B	344/362 (95%)	0.94	56 (16%) 2 2	16, 31, 46, 53	344 (100%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	13-A	337/362 (93%)	1.21	81 (24%)	1	1	15, 33, 53, 80	337 (100%)
1	13-B	344/362 (95%)	0.94	56 (16%)	2	2	16, 31, 46, 53	344 (100%)
1	14-A	337/362 (93%)	1.21	81 (24%)	1	1	15, 33, 53, 80	337 (100%)
1	14-B	344/362 (95%)	0.94	56 (16%)	2	2	16, 31, 46, 53	344 (100%)
1	15-A	337/362 (93%)	1.21	81 (24%)	1	1	15, 33, 53, 80	337 (100%)
1	15-B	344/362 (95%)	0.94	56 (16%)	2	2	16, 31, 46, 53	344 (100%)
1	16-A	337/362 (93%)	1.21	81 (24%)	1	1	15, 33, 53, 80	337 (100%)
1	16-B	344/362 (95%)	0.94	56 (16%)	2	2	16, 31, 46, 53	344 (100%)
All	All	10896/11584 (94%)	1.07	2192 (20%)	2	1	15, 32, 51, 80	10896 (100%)

All (2192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	317	LEU	9.8
1	2-A	317	LEU	9.8
1	3-A	317	LEU	9.8
1	4-A	317	LEU	9.8
1	5-A	317	LEU	9.8
1	6-A	317	LEU	9.8
1	7-A	317	LEU	9.8
1	8-A	317	LEU	9.8
1	9-A	317	LEU	9.8
1	10-A	317	LEU	9.8
1	11-A	317	LEU	9.8
1	12-A	317	LEU	9.8
1	13-A	317	LEU	9.8
1	14-A	317	LEU	9.8
1	15-A	317	LEU	9.8
1	16-A	317	LEU	9.8
1	1-A	56	SER	6.8
1	2-A	56	SER	6.8
1	3-A	56	SER	6.8
1	4-A	56	SER	6.8
1	5-A	56	SER	6.8
1	6-A	56	SER	6.8
1	7-A	56	SER	6.8
1	8-A	56	SER	6.8
1	9-A	56	SER	6.8
1	10-A	56	SER	6.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	11-A	56	SER	6.8
1	12-A	56	SER	6.8
1	13-A	56	SER	6.8
1	14-A	56	SER	6.8
1	15-A	56	SER	6.8
1	16-A	56	SER	6.8
1	1-A	49	THR	6.6
1	2-A	49	THR	6.6
1	3-A	49	THR	6.6
1	4-A	49	THR	6.6
1	5-A	49	THR	6.6
1	6-A	49	THR	6.6
1	7-A	49	THR	6.6
1	8-A	49	THR	6.6
1	9-A	49	THR	6.6
1	10-A	49	THR	6.6
1	11-A	49	THR	6.6
1	12-A	49	THR	6.6
1	13-A	49	THR	6.6
1	14-A	49	THR	6.6
1	15-A	49	THR	6.6
1	16-A	49	THR	6.6
1	1-A	70	PRO	6.4
1	2-A	70	PRO	6.4
1	3-A	70	PRO	6.4
1	4-A	70	PRO	6.4
1	5-A	70	PRO	6.4
1	6-A	70	PRO	6.4
1	7-A	70	PRO	6.4
1	8-A	70	PRO	6.4
1	9-A	70	PRO	6.4
1	10-A	70	PRO	6.4
1	11-A	70	PRO	6.4
1	12-A	70	PRO	6.4
1	13-A	70	PRO	6.4
1	14-A	70	PRO	6.4
1	15-A	70	PRO	6.4
1	16-A	70	PRO	6.4
1	1-B	41	LEU	6.3
1	2-B	41	LEU	6.3
1	3-B	41	LEU	6.3
1	4-B	41	LEU	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	5-B	41	LEU	6.3
1	6-B	41	LEU	6.3
1	7-B	41	LEU	6.3
1	8-B	41	LEU	6.3
1	9-B	41	LEU	6.3
1	10-B	41	LEU	6.3
1	11-B	41	LEU	6.3
1	12-B	41	LEU	6.3
1	13-B	41	LEU	6.3
1	14-B	41	LEU	6.3
1	15-B	41	LEU	6.3
1	16-B	41	LEU	6.3
1	1-A	57	THR	6.3
1	2-A	57	THR	6.3
1	3-A	57	THR	6.3
1	4-A	57	THR	6.3
1	5-A	57	THR	6.3
1	6-A	57	THR	6.3
1	7-A	57	THR	6.3
1	8-A	57	THR	6.3
1	9-A	57	THR	6.3
1	10-A	57	THR	6.3
1	11-A	57	THR	6.3
1	12-A	57	THR	6.3
1	13-A	57	THR	6.3
1	14-A	57	THR	6.3
1	15-A	57	THR	6.3
1	16-A	57	THR	6.3
1	1-B	300	VAL	6.3
1	2-B	300	VAL	6.3
1	3-B	300	VAL	6.3
1	4-B	300	VAL	6.3
1	5-B	300	VAL	6.3
1	6-B	300	VAL	6.3
1	7-B	300	VAL	6.3
1	8-B	300	VAL	6.3
1	9-B	300	VAL	6.3
1	10-B	300	VAL	6.3
1	11-B	300	VAL	6.3
1	12-B	300	VAL	6.3
1	13-B	300	VAL	6.3
1	14-B	300	VAL	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	15-B	300	VAL	6.3
1	16-B	300	VAL	6.3
1	1-A	47	PHE	6.1
1	2-A	47	PHE	6.1
1	3-A	47	PHE	6.1
1	4-A	47	PHE	6.1
1	5-A	47	PHE	6.1
1	6-A	47	PHE	6.1
1	7-A	47	PHE	6.1
1	8-A	47	PHE	6.1
1	9-A	47	PHE	6.1
1	10-A	47	PHE	6.1
1	11-A	47	PHE	6.1
1	12-A	47	PHE	6.1
1	13-A	47	PHE	6.1
1	14-A	47	PHE	6.1
1	15-A	47	PHE	6.1
1	16-A	47	PHE	6.1
1	1-B	326	ALA	5.9
1	2-B	326	ALA	5.9
1	3-B	326	ALA	5.9
1	4-B	326	ALA	5.9
1	5-B	326	ALA	5.9
1	6-B	326	ALA	5.9
1	7-B	326	ALA	5.9
1	8-B	326	ALA	5.9
1	9-B	326	ALA	5.9
1	10-B	326	ALA	5.9
1	11-B	326	ALA	5.9
1	12-B	326	ALA	5.9
1	13-B	326	ALA	5.9
1	14-B	326	ALA	5.9
1	15-B	326	ALA	5.9
1	16-B	326	ALA	5.9
1	1-A	148	GLU	5.8
1	2-A	148	GLU	5.8
1	3-A	148	GLU	5.8
1	4-A	148	GLU	5.8
1	5-A	148	GLU	5.8
1	6-A	148	GLU	5.8
1	7-A	148	GLU	5.8
1	8-A	148	GLU	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	9-A	148	GLU	5.8
1	10-A	148	GLU	5.8
1	11-A	148	GLU	5.8
1	12-A	148	GLU	5.8
1	13-A	148	GLU	5.8
1	14-A	148	GLU	5.8
1	15-A	148	GLU	5.8
1	16-A	148	GLU	5.8
1	1-A	46	ALA	5.8
1	2-A	46	ALA	5.8
1	3-A	46	ALA	5.8
1	4-A	46	ALA	5.8
1	5-A	46	ALA	5.8
1	6-A	46	ALA	5.8
1	7-A	46	ALA	5.8
1	8-A	46	ALA	5.8
1	9-A	46	ALA	5.8
1	10-A	46	ALA	5.8
1	11-A	46	ALA	5.8
1	12-A	46	ALA	5.8
1	13-A	46	ALA	5.8
1	14-A	46	ALA	5.8
1	15-A	46	ALA	5.8
1	16-A	46	ALA	5.8
1	1-A	45	LYS	5.7
1	2-A	45	LYS	5.7
1	3-A	45	LYS	5.7
1	4-A	45	LYS	5.7
1	5-A	45	LYS	5.7
1	6-A	45	LYS	5.7
1	7-A	45	LYS	5.7
1	8-A	45	LYS	5.7
1	9-A	45	LYS	5.7
1	10-A	45	LYS	5.7
1	11-A	45	LYS	5.7
1	12-A	45	LYS	5.7
1	13-A	45	LYS	5.7
1	14-A	45	LYS	5.7
1	15-A	45	LYS	5.7
1	16-A	45	LYS	5.7
1	1-A	315	ALA	5.6
1	2-A	315	ALA	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	3-A	315	ALA	5.6
1	4-A	315	ALA	5.6
1	5-A	315	ALA	5.6
1	6-A	315	ALA	5.6
1	7-A	315	ALA	5.6
1	8-A	315	ALA	5.6
1	9-A	315	ALA	5.6
1	10-A	315	ALA	5.6
1	11-A	315	ALA	5.6
1	12-A	315	ALA	5.6
1	13-A	315	ALA	5.6
1	14-A	315	ALA	5.6
1	15-A	315	ALA	5.6
1	16-A	315	ALA	5.6
1	1-B	324	ASN	5.4
1	2-B	324	ASN	5.4
1	3-B	324	ASN	5.4
1	4-B	324	ASN	5.4
1	5-B	324	ASN	5.4
1	6-B	324	ASN	5.4
1	7-B	324	ASN	5.4
1	8-B	324	ASN	5.4
1	9-B	324	ASN	5.4
1	10-B	324	ASN	5.4
1	11-B	324	ASN	5.4
1	12-B	324	ASN	5.4
1	13-B	324	ASN	5.4
1	14-B	324	ASN	5.4
1	15-B	324	ASN	5.4
1	16-B	324	ASN	5.4
1	1-B	274	ALA	5.4
1	2-B	274	ALA	5.4
1	3-B	274	ALA	5.4
1	4-B	274	ALA	5.4
1	5-B	274	ALA	5.4
1	6-B	274	ALA	5.4
1	7-B	274	ALA	5.4
1	8-B	274	ALA	5.4
1	9-B	274	ALA	5.4
1	10-B	274	ALA	5.4
1	11-B	274	ALA	5.4
1	12-B	274	ALA	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	13-B	274	ALA	5.4
1	14-B	274	ALA	5.4
1	15-B	274	ALA	5.4
1	16-B	274	ALA	5.4
1	1-B	321	ILE	5.2
1	2-B	321	ILE	5.2
1	3-B	321	ILE	5.2
1	4-B	321	ILE	5.2
1	5-B	321	ILE	5.2
1	6-B	321	ILE	5.2
1	7-B	321	ILE	5.2
1	8-B	321	ILE	5.2
1	9-B	321	ILE	5.2
1	10-B	321	ILE	5.2
1	11-B	321	ILE	5.2
1	12-B	321	ILE	5.2
1	13-B	321	ILE	5.2
1	14-B	321	ILE	5.2
1	15-B	321	ILE	5.2
1	16-B	321	ILE	5.2
1	1-A	167	ASP	5.2
1	2-A	167	ASP	5.2
1	3-A	167	ASP	5.2
1	4-A	167	ASP	5.2
1	5-A	167	ASP	5.2
1	6-A	167	ASP	5.2
1	7-A	167	ASP	5.2
1	8-A	167	ASP	5.2
1	9-A	167	ASP	5.2
1	10-A	167	ASP	5.2
1	11-A	167	ASP	5.2
1	12-A	167	ASP	5.2
1	13-A	167	ASP	5.2
1	14-A	167	ASP	5.2
1	15-A	167	ASP	5.2
1	16-A	167	ASP	5.2
1	1-B	325	GLY	5.1
1	2-B	325	GLY	5.1
1	3-B	325	GLY	5.1
1	4-B	325	GLY	5.1
1	5-B	325	GLY	5.1
1	6-B	325	GLY	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	7-B	325	GLY	5.1
1	8-B	325	GLY	5.1
1	9-B	325	GLY	5.1
1	10-B	325	GLY	5.1
1	11-B	325	GLY	5.1
1	12-B	325	GLY	5.1
1	13-B	325	GLY	5.1
1	14-B	325	GLY	5.1
1	15-B	325	GLY	5.1
1	16-B	325	GLY	5.1
1	1-B	28	ALA	5.1
1	2-B	28	ALA	5.1
1	3-B	28	ALA	5.1
1	4-B	28	ALA	5.1
1	5-B	28	ALA	5.1
1	6-B	28	ALA	5.1
1	7-B	28	ALA	5.1
1	8-B	28	ALA	5.1
1	9-B	28	ALA	5.1
1	10-B	28	ALA	5.1
1	11-B	28	ALA	5.1
1	12-B	28	ALA	5.1
1	13-B	28	ALA	5.1
1	14-B	28	ALA	5.1
1	15-B	28	ALA	5.1
1	16-B	28	ALA	5.1
1	1-A	55	GLU	5.0
1	2-A	55	GLU	5.0
1	3-A	55	GLU	5.0
1	4-A	55	GLU	5.0
1	5-A	55	GLU	5.0
1	6-A	55	GLU	5.0
1	7-A	55	GLU	5.0
1	8-A	55	GLU	5.0
1	9-A	55	GLU	5.0
1	10-A	55	GLU	5.0
1	11-A	55	GLU	5.0
1	12-A	55	GLU	5.0
1	13-A	55	GLU	5.0
1	14-A	55	GLU	5.0
1	15-A	55	GLU	5.0
1	16-A	55	GLU	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-A	165	ASP	4.9
1	2-A	165	ASP	4.9
1	3-A	165	ASP	4.9
1	4-A	165	ASP	4.9
1	5-A	165	ASP	4.9
1	6-A	165	ASP	4.9
1	7-A	165	ASP	4.9
1	8-A	165	ASP	4.9
1	9-A	165	ASP	4.9
1	10-A	165	ASP	4.9
1	11-A	165	ASP	4.9
1	12-A	165	ASP	4.9
1	13-A	165	ASP	4.9
1	14-A	165	ASP	4.9
1	15-A	165	ASP	4.9
1	16-A	165	ASP	4.9
1	1-B	40	SER	4.7
1	2-B	40	SER	4.7
1	3-B	40	SER	4.7
1	4-B	40	SER	4.7
1	5-B	40	SER	4.7
1	6-B	40	SER	4.7
1	7-B	40	SER	4.7
1	8-B	40	SER	4.7
1	9-B	40	SER	4.7
1	10-B	40	SER	4.7
1	11-B	40	SER	4.7
1	12-B	40	SER	4.7
1	13-B	40	SER	4.7
1	14-B	40	SER	4.7
1	15-B	40	SER	4.7
1	16-B	40	SER	4.7
1	1-B	353	ASN	4.6
1	2-B	353	ASN	4.6
1	3-B	353	ASN	4.6
1	4-B	353	ASN	4.6
1	5-B	353	ASN	4.6
1	6-B	353	ASN	4.6
1	7-B	353	ASN	4.6
1	8-B	353	ASN	4.6
1	9-B	353	ASN	4.6
1	10-B	353	ASN	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	11-B	353	ASN	4.6
1	12-B	353	ASN	4.6
1	13-B	353	ASN	4.6
1	14-B	353	ASN	4.6
1	15-B	353	ASN	4.6
1	16-B	353	ASN	4.6
1	1-A	33	ILE	4.5
1	2-A	33	ILE	4.5
1	3-A	33	ILE	4.5
1	4-A	33	ILE	4.5
1	5-A	33	ILE	4.5
1	6-A	33	ILE	4.5
1	7-A	33	ILE	4.5
1	8-A	33	ILE	4.5
1	9-A	33	ILE	4.5
1	10-A	33	ILE	4.5
1	11-A	33	ILE	4.5
1	12-A	33	ILE	4.5
1	13-A	33	ILE	4.5
1	14-A	33	ILE	4.5
1	15-A	33	ILE	4.5
1	16-A	33	ILE	4.5
1	1-A	66	LEU	4.5
1	2-A	66	LEU	4.5
1	3-A	66	LEU	4.5
1	4-A	66	LEU	4.5
1	5-A	66	LEU	4.5
1	6-A	66	LEU	4.5
1	7-A	66	LEU	4.5
1	8-A	66	LEU	4.5
1	9-A	66	LEU	4.5
1	10-A	66	LEU	4.5
1	11-A	66	LEU	4.5
1	12-A	66	LEU	4.5
1	13-A	66	LEU	4.5
1	14-A	66	LEU	4.5
1	15-A	66	LEU	4.5
1	16-A	66	LEU	4.5
1	1-A	300	VAL	4.4
1	2-A	300	VAL	4.4
1	3-A	300	VAL	4.4
1	4-A	300	VAL	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	5-A	300	VAL	4.4
1	6-A	300	VAL	4.4
1	7-A	300	VAL	4.4
1	8-A	300	VAL	4.4
1	9-A	300	VAL	4.4
1	10-A	300	VAL	4.4
1	11-A	300	VAL	4.4
1	12-A	300	VAL	4.4
1	13-A	300	VAL	4.4
1	14-A	300	VAL	4.4
1	15-A	300	VAL	4.4
1	16-A	300	VAL	4.4
1	1-A	14	CYS	4.2
1	2-A	14	CYS	4.2
1	3-A	14	CYS	4.2
1	4-A	14	CYS	4.2
1	5-A	14	CYS	4.2
1	6-A	14	CYS	4.2
1	7-A	14	CYS	4.2
1	8-A	14	CYS	4.2
1	9-A	14	CYS	4.2
1	10-A	14	CYS	4.2
1	11-A	14	CYS	4.2
1	12-A	14	CYS	4.2
1	13-A	14	CYS	4.2
1	14-A	14	CYS	4.2
1	15-A	14	CYS	4.2
1	16-A	14	CYS	4.2
1	1-A	109	THR	4.1
1	1-B	272	THR	4.1
1	2-A	109	THR	4.1
1	2-B	272	THR	4.1
1	3-A	109	THR	4.1
1	3-B	272	THR	4.1
1	4-A	109	THR	4.1
1	4-B	272	THR	4.1
1	5-A	109	THR	4.1
1	5-B	272	THR	4.1
1	6-A	109	THR	4.1
1	6-B	272	THR	4.1
1	7-A	109	THR	4.1
1	7-B	272	THR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	8-A	109	THR	4.1
1	8-B	272	THR	4.1
1	9-A	109	THR	4.1
1	9-B	272	THR	4.1
1	10-A	109	THR	4.1
1	10-B	272	THR	4.1
1	11-A	109	THR	4.1
1	11-B	272	THR	4.1
1	12-A	109	THR	4.1
1	12-B	272	THR	4.1
1	13-A	109	THR	4.1
1	13-B	272	THR	4.1
1	14-A	109	THR	4.1
1	14-B	272	THR	4.1
1	15-A	109	THR	4.1
1	15-B	272	THR	4.1
1	16-A	109	THR	4.1
1	16-B	272	THR	4.1
1	1-A	283	TRP	4.1
1	2-A	283	TRP	4.1
1	3-A	283	TRP	4.1
1	4-A	283	TRP	4.1
1	5-A	283	TRP	4.1
1	6-A	283	TRP	4.1
1	7-A	283	TRP	4.1
1	8-A	283	TRP	4.1
1	9-A	283	TRP	4.1
1	10-A	283	TRP	4.1
1	11-A	283	TRP	4.1
1	12-A	283	TRP	4.1
1	13-A	283	TRP	4.1
1	14-A	283	TRP	4.1
1	15-A	283	TRP	4.1
1	16-A	283	TRP	4.1
1	1-A	299	THR	4.1
1	2-A	299	THR	4.1
1	3-A	299	THR	4.1
1	4-A	299	THR	4.1
1	5-A	299	THR	4.1
1	6-A	299	THR	4.1
1	7-A	299	THR	4.1
1	8-A	299	THR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	9-A	299	THR	4.1
1	10-A	299	THR	4.1
1	11-A	299	THR	4.1
1	12-A	299	THR	4.1
1	13-A	299	THR	4.1
1	14-A	299	THR	4.1
1	15-A	299	THR	4.1
1	16-A	299	THR	4.1
1	1-B	85	VAL	4.0
1	2-B	85	VAL	4.0
1	3-B	85	VAL	4.0
1	4-B	85	VAL	4.0
1	5-B	85	VAL	4.0
1	6-B	85	VAL	4.0
1	7-B	85	VAL	4.0
1	8-B	85	VAL	4.0
1	9-B	85	VAL	4.0
1	10-B	85	VAL	4.0
1	11-B	85	VAL	4.0
1	12-B	85	VAL	4.0
1	13-B	85	VAL	4.0
1	14-B	85	VAL	4.0
1	15-B	85	VAL	4.0
1	16-B	85	VAL	4.0
1	1-A	58	LYS	4.0
1	2-A	58	LYS	4.0
1	3-A	58	LYS	4.0
1	4-A	58	LYS	4.0
1	5-A	58	LYS	4.0
1	6-A	58	LYS	4.0
1	7-A	58	LYS	4.0
1	8-A	58	LYS	4.0
1	9-A	58	LYS	4.0
1	10-A	58	LYS	4.0
1	11-A	58	LYS	4.0
1	12-A	58	LYS	4.0
1	13-A	58	LYS	4.0
1	14-A	58	LYS	4.0
1	15-A	58	LYS	4.0
1	16-A	58	LYS	4.0
1	1-B	167	ASP	4.0
1	2-B	167	ASP	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	3-B	167	ASP	4.0
1	4-B	167	ASP	4.0
1	5-B	167	ASP	4.0
1	6-B	167	ASP	4.0
1	7-B	167	ASP	4.0
1	8-B	167	ASP	4.0
1	9-B	167	ASP	4.0
1	10-B	167	ASP	4.0
1	11-B	167	ASP	4.0
1	12-B	167	ASP	4.0
1	13-B	167	ASP	4.0
1	14-B	167	ASP	4.0
1	15-B	167	ASP	4.0
1	16-B	167	ASP	4.0
1	1-A	42	GLU	3.9
1	2-A	42	GLU	3.9
1	3-A	42	GLU	3.9
1	4-A	42	GLU	3.9
1	5-A	42	GLU	3.9
1	6-A	42	GLU	3.9
1	7-A	42	GLU	3.9
1	8-A	42	GLU	3.9
1	9-A	42	GLU	3.9
1	10-A	42	GLU	3.9
1	11-A	42	GLU	3.9
1	12-A	42	GLU	3.9
1	13-A	42	GLU	3.9
1	14-A	42	GLU	3.9
1	15-A	42	GLU	3.9
1	16-A	42	GLU	3.9
1	1-A	206	LYS	3.9
1	2-A	206	LYS	3.9
1	3-A	206	LYS	3.9
1	4-A	206	LYS	3.9
1	5-A	206	LYS	3.9
1	6-A	206	LYS	3.9
1	7-A	206	LYS	3.9
1	8-A	206	LYS	3.9
1	9-A	206	LYS	3.9
1	10-A	206	LYS	3.9
1	11-A	206	LYS	3.9
1	12-A	206	LYS	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	13-A	206	LYS	3.9
1	14-A	206	LYS	3.9
1	15-A	206	LYS	3.9
1	16-A	206	LYS	3.9
1	1-B	220	GLY	3.9
1	2-B	220	GLY	3.9
1	3-B	220	GLY	3.9
1	4-B	220	GLY	3.9
1	5-B	220	GLY	3.9
1	6-B	220	GLY	3.9
1	7-B	220	GLY	3.9
1	8-B	220	GLY	3.9
1	9-B	220	GLY	3.9
1	10-B	220	GLY	3.9
1	11-B	220	GLY	3.9
1	12-B	220	GLY	3.9
1	13-B	220	GLY	3.9
1	14-B	220	GLY	3.9
1	15-B	220	GLY	3.9
1	16-B	220	GLY	3.9
1	1-A	30	ASN	3.8
1	2-A	30	ASN	3.8
1	3-A	30	ASN	3.8
1	4-A	30	ASN	3.8
1	5-A	30	ASN	3.8
1	6-A	30	ASN	3.8
1	7-A	30	ASN	3.8
1	8-A	30	ASN	3.8
1	9-A	30	ASN	3.8
1	10-A	30	ASN	3.8
1	11-A	30	ASN	3.8
1	12-A	30	ASN	3.8
1	13-A	30	ASN	3.8
1	14-A	30	ASN	3.8
1	15-A	30	ASN	3.8
1	16-A	30	ASN	3.8
1	1-B	39	ARG	3.8
1	2-B	39	ARG	3.8
1	3-B	39	ARG	3.8
1	4-B	39	ARG	3.8
1	5-B	39	ARG	3.8
1	6-B	39	ARG	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	7-B	39	ARG	3.8
1	8-B	39	ARG	3.8
1	9-B	39	ARG	3.8
1	10-B	39	ARG	3.8
1	11-B	39	ARG	3.8
1	12-B	39	ARG	3.8
1	13-B	39	ARG	3.8
1	14-B	39	ARG	3.8
1	15-B	39	ARG	3.8
1	16-B	39	ARG	3.8
1	1-B	171	ASN	3.8
1	2-B	171	ASN	3.8
1	3-B	171	ASN	3.8
1	4-B	171	ASN	3.8
1	5-B	171	ASN	3.8
1	6-B	171	ASN	3.8
1	7-B	171	ASN	3.8
1	8-B	171	ASN	3.8
1	9-B	171	ASN	3.8
1	10-B	171	ASN	3.8
1	11-B	171	ASN	3.8
1	12-B	171	ASN	3.8
1	13-B	171	ASN	3.8
1	14-B	171	ASN	3.8
1	15-B	171	ASN	3.8
1	16-B	171	ASN	3.8
1	1-B	166	GLU	3.7
1	2-B	166	GLU	3.7
1	3-B	166	GLU	3.7
1	4-B	166	GLU	3.7
1	5-B	166	GLU	3.7
1	6-B	166	GLU	3.7
1	7-B	166	GLU	3.7
1	8-B	166	GLU	3.7
1	9-B	166	GLU	3.7
1	10-B	166	GLU	3.7
1	11-B	166	GLU	3.7
1	12-B	166	GLU	3.7
1	13-B	166	GLU	3.7
1	14-B	166	GLU	3.7
1	15-B	166	GLU	3.7
1	16-B	166	GLU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-A	29	PRO	3.7
1	2-A	29	PRO	3.7
1	3-A	29	PRO	3.7
1	4-A	29	PRO	3.7
1	5-A	29	PRO	3.7
1	6-A	29	PRO	3.7
1	7-A	29	PRO	3.7
1	8-A	29	PRO	3.7
1	9-A	29	PRO	3.7
1	10-A	29	PRO	3.7
1	11-A	29	PRO	3.7
1	12-A	29	PRO	3.7
1	13-A	29	PRO	3.7
1	14-A	29	PRO	3.7
1	15-A	29	PRO	3.7
1	16-A	29	PRO	3.7
1	1-B	273	GLU	3.7
1	2-B	273	GLU	3.7
1	3-B	273	GLU	3.7
1	4-B	273	GLU	3.7
1	5-B	273	GLU	3.7
1	6-B	273	GLU	3.7
1	7-B	273	GLU	3.7
1	8-B	273	GLU	3.7
1	9-B	273	GLU	3.7
1	10-B	273	GLU	3.7
1	11-B	273	GLU	3.7
1	12-B	273	GLU	3.7
1	13-B	273	GLU	3.7
1	14-B	273	GLU	3.7
1	15-B	273	GLU	3.7
1	16-B	273	GLU	3.7
1	1-A	54	PRO	3.7
1	2-A	54	PRO	3.7
1	3-A	54	PRO	3.7
1	4-A	54	PRO	3.7
1	5-A	54	PRO	3.7
1	6-A	54	PRO	3.7
1	7-A	54	PRO	3.7
1	8-A	54	PRO	3.7
1	9-A	54	PRO	3.7
1	10-A	54	PRO	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	11-A	54	PRO	3.7
1	12-A	54	PRO	3.7
1	13-A	54	PRO	3.7
1	14-A	54	PRO	3.7
1	15-A	54	PRO	3.7
1	16-A	54	PRO	3.7
1	1-A	331	TYR	3.7
1	2-A	331	TYR	3.7
1	3-A	331	TYR	3.7
1	4-A	331	TYR	3.7
1	5-A	331	TYR	3.7
1	6-A	331	TYR	3.7
1	7-A	331	TYR	3.7
1	8-A	331	TYR	3.7
1	9-A	331	TYR	3.7
1	10-A	331	TYR	3.7
1	11-A	331	TYR	3.7
1	12-A	331	TYR	3.7
1	13-A	331	TYR	3.7
1	14-A	331	TYR	3.7
1	15-A	331	TYR	3.7
1	16-A	331	TYR	3.7
1	1-B	6	GLN	3.6
1	2-B	6	GLN	3.6
1	3-B	6	GLN	3.6
1	4-B	6	GLN	3.6
1	5-B	6	GLN	3.6
1	6-B	6	GLN	3.6
1	7-B	6	GLN	3.6
1	8-B	6	GLN	3.6
1	9-B	6	GLN	3.6
1	10-B	6	GLN	3.6
1	11-B	6	GLN	3.6
1	12-B	6	GLN	3.6
1	13-B	6	GLN	3.6
1	14-B	6	GLN	3.6
1	15-B	6	GLN	3.6
1	16-B	6	GLN	3.6
1	1-B	315	ALA	3.6
1	2-B	315	ALA	3.6
1	3-B	315	ALA	3.6
1	4-B	315	ALA	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	5-B	315	ALA	3.6
1	6-B	315	ALA	3.6
1	7-B	315	ALA	3.6
1	8-B	315	ALA	3.6
1	9-B	315	ALA	3.6
1	10-B	315	ALA	3.6
1	11-B	315	ALA	3.6
1	12-B	315	ALA	3.6
1	13-B	315	ALA	3.6
1	14-B	315	ALA	3.6
1	15-B	315	ALA	3.6
1	16-B	315	ALA	3.6
1	1-A	40	SER	3.6
1	2-A	40	SER	3.6
1	3-A	40	SER	3.6
1	4-A	40	SER	3.6
1	5-A	40	SER	3.6
1	6-A	40	SER	3.6
1	7-A	40	SER	3.6
1	8-A	40	SER	3.6
1	9-A	40	SER	3.6
1	10-A	40	SER	3.6
1	11-A	40	SER	3.6
1	12-A	40	SER	3.6
1	13-A	40	SER	3.6
1	14-A	40	SER	3.6
1	15-A	40	SER	3.6
1	16-A	40	SER	3.6
1	1-A	71	GLU	3.6
1	2-A	71	GLU	3.6
1	3-A	71	GLU	3.6
1	4-A	71	GLU	3.6
1	5-A	71	GLU	3.6
1	6-A	71	GLU	3.6
1	7-A	71	GLU	3.6
1	8-A	71	GLU	3.6
1	9-A	71	GLU	3.6
1	10-A	71	GLU	3.6
1	11-A	71	GLU	3.6
1	12-A	71	GLU	3.6
1	13-A	71	GLU	3.6
1	14-A	71	GLU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	15-A	71	GLU	3.6
1	16-A	71	GLU	3.6
1	1-A	233	ASP	3.5
1	2-A	233	ASP	3.5
1	3-A	233	ASP	3.5
1	4-A	233	ASP	3.5
1	5-A	233	ASP	3.5
1	6-A	233	ASP	3.5
1	7-A	233	ASP	3.5
1	8-A	233	ASP	3.5
1	9-A	233	ASP	3.5
1	10-A	233	ASP	3.5
1	11-A	233	ASP	3.5
1	12-A	233	ASP	3.5
1	13-A	233	ASP	3.5
1	14-A	233	ASP	3.5
1	15-A	233	ASP	3.5
1	16-A	233	ASP	3.5
1	1-A	39	ARG	3.5
1	2-A	39	ARG	3.5
1	3-A	39	ARG	3.5
1	4-A	39	ARG	3.5
1	5-A	39	ARG	3.5
1	6-A	39	ARG	3.5
1	7-A	39	ARG	3.5
1	8-A	39	ARG	3.5
1	9-A	39	ARG	3.5
1	10-A	39	ARG	3.5
1	11-A	39	ARG	3.5
1	12-A	39	ARG	3.5
1	13-A	39	ARG	3.5
1	14-A	39	ARG	3.5
1	15-A	39	ARG	3.5
1	16-A	39	ARG	3.5
1	1-A	318	VAL	3.5
1	2-A	318	VAL	3.5
1	3-A	318	VAL	3.5
1	4-A	318	VAL	3.5
1	5-A	318	VAL	3.5
1	6-A	318	VAL	3.5
1	7-A	318	VAL	3.5
1	8-A	318	VAL	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	9-A	318	VAL	3.5
1	10-A	318	VAL	3.5
1	11-A	318	VAL	3.5
1	12-A	318	VAL	3.5
1	13-A	318	VAL	3.5
1	14-A	318	VAL	3.5
1	15-A	318	VAL	3.5
1	16-A	318	VAL	3.5
1	1-A	43	LYS	3.4
1	2-A	43	LYS	3.4
1	3-A	43	LYS	3.4
1	4-A	43	LYS	3.4
1	5-A	43	LYS	3.4
1	6-A	43	LYS	3.4
1	7-A	43	LYS	3.4
1	8-A	43	LYS	3.4
1	9-A	43	LYS	3.4
1	10-A	43	LYS	3.4
1	11-A	43	LYS	3.4
1	12-A	43	LYS	3.4
1	13-A	43	LYS	3.4
1	14-A	43	LYS	3.4
1	15-A	43	LYS	3.4
1	16-A	43	LYS	3.4
1	1-A	50	ALA	3.4
1	2-A	50	ALA	3.4
1	3-A	50	ALA	3.4
1	4-A	50	ALA	3.4
1	5-A	50	ALA	3.4
1	6-A	50	ALA	3.4
1	7-A	50	ALA	3.4
1	8-A	50	ALA	3.4
1	9-A	50	ALA	3.4
1	10-A	50	ALA	3.4
1	11-A	50	ALA	3.4
1	12-A	50	ALA	3.4
1	13-A	50	ALA	3.4
1	14-A	50	ALA	3.4
1	15-A	50	ALA	3.4
1	16-A	50	ALA	3.4
1	1-A	304	LEU	3.4
1	2-A	304	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	3-A	304	LEU	3.4
1	4-A	304	LEU	3.4
1	5-A	304	LEU	3.4
1	6-A	304	LEU	3.4
1	7-A	304	LEU	3.4
1	8-A	304	LEU	3.4
1	9-A	304	LEU	3.4
1	10-A	304	LEU	3.4
1	11-A	304	LEU	3.4
1	12-A	304	LEU	3.4
1	13-A	304	LEU	3.4
1	14-A	304	LEU	3.4
1	15-A	304	LEU	3.4
1	16-A	304	LEU	3.4
1	1-A	311	VAL	3.3
1	2-A	311	VAL	3.3
1	3-A	311	VAL	3.3
1	4-A	311	VAL	3.3
1	5-A	311	VAL	3.3
1	6-A	311	VAL	3.3
1	7-A	311	VAL	3.3
1	8-A	311	VAL	3.3
1	9-A	311	VAL	3.3
1	10-A	311	VAL	3.3
1	11-A	311	VAL	3.3
1	12-A	311	VAL	3.3
1	13-A	311	VAL	3.3
1	14-A	311	VAL	3.3
1	15-A	311	VAL	3.3
1	16-A	311	VAL	3.3
1	1-B	64	GLU	3.3
1	2-B	64	GLU	3.3
1	3-B	64	GLU	3.3
1	4-B	64	GLU	3.3
1	5-B	64	GLU	3.3
1	6-B	64	GLU	3.3
1	7-B	64	GLU	3.3
1	8-B	64	GLU	3.3
1	9-B	64	GLU	3.3
1	10-B	64	GLU	3.3
1	11-B	64	GLU	3.3
1	12-B	64	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	13-B	64	GLU	3.3
1	14-B	64	GLU	3.3
1	15-B	64	GLU	3.3
1	16-B	64	GLU	3.3
1	1-A	48	ALA	3.3
1	2-A	48	ALA	3.3
1	3-A	48	ALA	3.3
1	4-A	48	ALA	3.3
1	5-A	48	ALA	3.3
1	6-A	48	ALA	3.3
1	7-A	48	ALA	3.3
1	8-A	48	ALA	3.3
1	9-A	48	ALA	3.3
1	10-A	48	ALA	3.3
1	11-A	48	ALA	3.3
1	12-A	48	ALA	3.3
1	13-A	48	ALA	3.3
1	14-A	48	ALA	3.3
1	15-A	48	ALA	3.3
1	16-A	48	ALA	3.3
1	1-B	352	LYS	3.2
1	2-B	352	LYS	3.2
1	3-B	352	LYS	3.2
1	4-B	352	LYS	3.2
1	5-B	352	LYS	3.2
1	6-B	352	LYS	3.2
1	7-B	352	LYS	3.2
1	8-B	352	LYS	3.2
1	9-B	352	LYS	3.2
1	10-B	352	LYS	3.2
1	11-B	352	LYS	3.2
1	12-B	352	LYS	3.2
1	13-B	352	LYS	3.2
1	14-B	352	LYS	3.2
1	15-B	352	LYS	3.2
1	16-B	352	LYS	3.2
1	1-B	285	ASN	3.2
1	2-B	285	ASN	3.2
1	3-B	285	ASN	3.2
1	4-B	285	ASN	3.2
1	5-B	285	ASN	3.2
1	6-B	285	ASN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	7-B	285	ASN	3.2
1	8-B	285	ASN	3.2
1	9-B	285	ASN	3.2
1	10-B	285	ASN	3.2
1	11-B	285	ASN	3.2
1	12-B	285	ASN	3.2
1	13-B	285	ASN	3.2
1	14-B	285	ASN	3.2
1	15-B	285	ASN	3.2
1	16-B	285	ASN	3.2
1	1-A	234	GLY	3.2
1	2-A	234	GLY	3.2
1	3-A	234	GLY	3.2
1	4-A	234	GLY	3.2
1	5-A	234	GLY	3.2
1	6-A	234	GLY	3.2
1	7-A	234	GLY	3.2
1	8-A	234	GLY	3.2
1	9-A	234	GLY	3.2
1	10-A	234	GLY	3.2
1	11-A	234	GLY	3.2
1	12-A	234	GLY	3.2
1	13-A	234	GLY	3.2
1	14-A	234	GLY	3.2
1	15-A	234	GLY	3.2
1	16-A	234	GLY	3.2
1	1-B	170	LYS	3.2
1	2-B	170	LYS	3.2
1	3-B	170	LYS	3.2
1	4-B	170	LYS	3.2
1	5-B	170	LYS	3.2
1	6-B	170	LYS	3.2
1	7-B	170	LYS	3.2
1	8-B	170	LYS	3.2
1	9-B	170	LYS	3.2
1	10-B	170	LYS	3.2
1	11-B	170	LYS	3.2
1	12-B	170	LYS	3.2
1	13-B	170	LYS	3.2
1	14-B	170	LYS	3.2
1	15-B	170	LYS	3.2
1	16-B	170	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-B	70	PRO	3.2
1	2-B	70	PRO	3.2
1	3-B	70	PRO	3.2
1	4-B	70	PRO	3.2
1	5-B	70	PRO	3.2
1	6-B	70	PRO	3.2
1	7-B	70	PRO	3.2
1	8-B	70	PRO	3.2
1	9-B	70	PRO	3.2
1	10-B	70	PRO	3.2
1	11-B	70	PRO	3.2
1	12-B	70	PRO	3.2
1	13-B	70	PRO	3.2
1	14-B	70	PRO	3.2
1	15-B	70	PRO	3.2
1	16-B	70	PRO	3.2
1	1-A	69	ASP	3.2
1	1-A	149	ARG	3.2
1	2-A	69	ASP	3.2
1	2-A	149	ARG	3.2
1	3-A	69	ASP	3.2
1	3-A	149	ARG	3.2
1	4-A	69	ASP	3.2
1	4-A	149	ARG	3.2
1	5-A	69	ASP	3.2
1	5-A	149	ARG	3.2
1	6-A	69	ASP	3.2
1	6-A	149	ARG	3.2
1	7-A	69	ASP	3.2
1	7-A	149	ARG	3.2
1	8-A	69	ASP	3.2
1	8-A	149	ARG	3.2
1	9-A	69	ASP	3.2
1	9-A	149	ARG	3.2
1	10-A	69	ASP	3.2
1	10-A	149	ARG	3.2
1	11-A	69	ASP	3.2
1	11-A	149	ARG	3.2
1	12-A	69	ASP	3.2
1	12-A	149	ARG	3.2
1	13-A	69	ASP	3.2
1	13-A	149	ARG	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	14-A	69	ASP	3.2
1	14-A	149	ARG	3.2
1	15-A	69	ASP	3.2
1	15-A	149	ARG	3.2
1	16-A	69	ASP	3.2
1	16-A	149	ARG	3.2
1	1-A	67	LEU	3.2
1	2-A	67	LEU	3.2
1	3-A	67	LEU	3.2
1	4-A	67	LEU	3.2
1	5-A	67	LEU	3.2
1	6-A	67	LEU	3.2
1	7-A	67	LEU	3.2
1	8-A	67	LEU	3.2
1	9-A	67	LEU	3.2
1	10-A	67	LEU	3.2
1	11-A	67	LEU	3.2
1	12-A	67	LEU	3.2
1	13-A	67	LEU	3.2
1	14-A	67	LEU	3.2
1	15-A	67	LEU	3.2
1	16-A	67	LEU	3.2
1	1-B	328	PRO	3.2
1	2-B	328	PRO	3.2
1	3-B	328	PRO	3.2
1	4-B	328	PRO	3.2
1	5-B	328	PRO	3.2
1	6-B	328	PRO	3.2
1	7-B	328	PRO	3.2
1	8-B	328	PRO	3.2
1	9-B	328	PRO	3.2
1	10-B	328	PRO	3.2
1	11-B	328	PRO	3.2
1	12-B	328	PRO	3.2
1	13-B	328	PRO	3.2
1	14-B	328	PRO	3.2
1	15-B	328	PRO	3.2
1	16-B	328	PRO	3.2
1	1-A	102	LYS	3.2
1	2-A	102	LYS	3.2
1	3-A	102	LYS	3.2
1	4-A	102	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	5-A	102	LYS	3.2
1	6-A	102	LYS	3.2
1	7-A	102	LYS	3.2
1	8-A	102	LYS	3.2
1	9-A	102	LYS	3.2
1	10-A	102	LYS	3.2
1	11-A	102	LYS	3.2
1	12-A	102	LYS	3.2
1	13-A	102	LYS	3.2
1	14-A	102	LYS	3.2
1	15-A	102	LYS	3.2
1	16-A	102	LYS	3.2
1	1-A	152	GLN	3.1
1	2-A	152	GLN	3.1
1	3-A	152	GLN	3.1
1	4-A	152	GLN	3.1
1	5-A	152	GLN	3.1
1	6-A	152	GLN	3.1
1	7-A	152	GLN	3.1
1	8-A	152	GLN	3.1
1	9-A	152	GLN	3.1
1	10-A	152	GLN	3.1
1	11-A	152	GLN	3.1
1	12-A	152	GLN	3.1
1	13-A	152	GLN	3.1
1	14-A	152	GLN	3.1
1	15-A	152	GLN	3.1
1	16-A	152	GLN	3.1
1	1-B	322	LYS	3.1
1	2-B	322	LYS	3.1
1	3-B	322	LYS	3.1
1	4-B	322	LYS	3.1
1	5-B	322	LYS	3.1
1	6-B	322	LYS	3.1
1	7-B	322	LYS	3.1
1	8-B	322	LYS	3.1
1	9-B	322	LYS	3.1
1	10-B	322	LYS	3.1
1	11-B	322	LYS	3.1
1	12-B	322	LYS	3.1
1	13-B	322	LYS	3.1
1	14-B	322	LYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	15-B	322	LYS	3.1
1	16-B	322	LYS	3.1
1	1-A	51	ASN	3.1
1	1-B	56	SER	3.1
1	2-A	51	ASN	3.1
1	2-B	56	SER	3.1
1	3-A	51	ASN	3.1
1	3-B	56	SER	3.1
1	4-A	51	ASN	3.1
1	4-B	56	SER	3.1
1	5-A	51	ASN	3.1
1	5-B	56	SER	3.1
1	6-A	51	ASN	3.1
1	6-B	56	SER	3.1
1	7-A	51	ASN	3.1
1	7-B	56	SER	3.1
1	8-A	51	ASN	3.1
1	8-B	56	SER	3.1
1	9-A	51	ASN	3.1
1	9-B	56	SER	3.1
1	10-A	51	ASN	3.1
1	10-B	56	SER	3.1
1	11-A	51	ASN	3.1
1	11-B	56	SER	3.1
1	12-A	51	ASN	3.1
1	12-B	56	SER	3.1
1	13-A	51	ASN	3.1
1	13-B	56	SER	3.1
1	14-A	51	ASN	3.1
1	14-B	56	SER	3.1
1	15-A	51	ASN	3.1
1	15-B	56	SER	3.1
1	16-A	51	ASN	3.1
1	16-B	56	SER	3.1
1	1-A	309	CYS	3.1
1	2-A	309	CYS	3.1
1	3-A	309	CYS	3.1
1	4-A	309	CYS	3.1
1	5-A	309	CYS	3.1
1	6-A	309	CYS	3.1
1	7-A	309	CYS	3.1
1	8-A	309	CYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	9-A	309	CYS	3.1
1	10-A	309	CYS	3.1
1	11-A	309	CYS	3.1
1	12-A	309	CYS	3.1
1	13-A	309	CYS	3.1
1	14-A	309	CYS	3.1
1	15-A	309	CYS	3.1
1	16-A	309	CYS	3.1
1	1-A	356	GLN	3.0
1	2-A	356	GLN	3.0
1	3-A	356	GLN	3.0
1	4-A	356	GLN	3.0
1	5-A	356	GLN	3.0
1	6-A	356	GLN	3.0
1	7-A	356	GLN	3.0
1	8-A	356	GLN	3.0
1	9-A	356	GLN	3.0
1	10-A	356	GLN	3.0
1	11-A	356	GLN	3.0
1	12-A	356	GLN	3.0
1	13-A	356	GLN	3.0
1	14-A	356	GLN	3.0
1	15-A	356	GLN	3.0
1	16-A	356	GLN	3.0
1	1-B	287	LEU	3.0
1	2-B	287	LEU	3.0
1	3-B	287	LEU	3.0
1	4-B	287	LEU	3.0
1	5-B	287	LEU	3.0
1	6-B	287	LEU	3.0
1	7-B	287	LEU	3.0
1	8-B	287	LEU	3.0
1	9-B	287	LEU	3.0
1	10-B	287	LEU	3.0
1	11-B	287	LEU	3.0
1	12-B	287	LEU	3.0
1	13-B	287	LEU	3.0
1	14-B	287	LEU	3.0
1	15-B	287	LEU	3.0
1	16-B	287	LEU	3.0
1	1-A	44	ALA	3.0
1	2-A	44	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	3-A	44	ALA	3.0
1	4-A	44	ALA	3.0
1	5-A	44	ALA	3.0
1	6-A	44	ALA	3.0
1	7-A	44	ALA	3.0
1	8-A	44	ALA	3.0
1	9-A	44	ALA	3.0
1	10-A	44	ALA	3.0
1	11-A	44	ALA	3.0
1	12-A	44	ALA	3.0
1	13-A	44	ALA	3.0
1	14-A	44	ALA	3.0
1	15-A	44	ALA	3.0
1	16-A	44	ALA	3.0
1	1-A	61	GLY	3.0
1	2-A	61	GLY	3.0
1	3-A	61	GLY	3.0
1	4-A	61	GLY	3.0
1	5-A	61	GLY	3.0
1	6-A	61	GLY	3.0
1	7-A	61	GLY	3.0
1	8-A	61	GLY	3.0
1	9-A	61	GLY	3.0
1	10-A	61	GLY	3.0
1	11-A	61	GLY	3.0
1	12-A	61	GLY	3.0
1	13-A	61	GLY	3.0
1	14-A	61	GLY	3.0
1	15-A	61	GLY	3.0
1	16-A	61	GLY	3.0
1	1-B	34	SER	2.9
1	2-B	34	SER	2.9
1	3-B	34	SER	2.9
1	4-B	34	SER	2.9
1	5-B	34	SER	2.9
1	6-B	34	SER	2.9
1	7-B	34	SER	2.9
1	8-B	34	SER	2.9
1	9-B	34	SER	2.9
1	10-B	34	SER	2.9
1	11-B	34	SER	2.9
1	12-B	34	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	13-B	34	SER	2.9
1	14-B	34	SER	2.9
1	15-B	34	SER	2.9
1	16-B	34	SER	2.9
1	1-B	169	LEU	2.8
1	2-B	169	LEU	2.8
1	3-B	169	LEU	2.8
1	4-B	169	LEU	2.8
1	5-B	169	LEU	2.8
1	6-B	169	LEU	2.8
1	7-B	169	LEU	2.8
1	8-B	169	LEU	2.8
1	9-B	169	LEU	2.8
1	10-B	169	LEU	2.8
1	11-B	169	LEU	2.8
1	12-B	169	LEU	2.8
1	13-B	169	LEU	2.8
1	14-B	169	LEU	2.8
1	15-B	169	LEU	2.8
1	16-B	169	LEU	2.8
1	1-B	271	GLU	2.8
1	2-B	271	GLU	2.8
1	3-B	271	GLU	2.8
1	4-B	271	GLU	2.8
1	5-B	271	GLU	2.8
1	6-B	271	GLU	2.8
1	7-B	271	GLU	2.8
1	8-B	271	GLU	2.8
1	9-B	271	GLU	2.8
1	10-B	271	GLU	2.8
1	11-B	271	GLU	2.8
1	12-B	271	GLU	2.8
1	13-B	271	GLU	2.8
1	14-B	271	GLU	2.8
1	15-B	271	GLU	2.8
1	16-B	271	GLU	2.8
1	1-B	42	GLU	2.8
1	2-B	42	GLU	2.8
1	3-B	42	GLU	2.8
1	4-B	42	GLU	2.8
1	5-B	42	GLU	2.8
1	6-B	42	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	7-B	42	GLU	2.8
1	8-B	42	GLU	2.8
1	9-B	42	GLU	2.8
1	10-B	42	GLU	2.8
1	11-B	42	GLU	2.8
1	12-B	42	GLU	2.8
1	13-B	42	GLU	2.8
1	14-B	42	GLU	2.8
1	15-B	42	GLU	2.8
1	16-B	42	GLU	2.8
1	1-A	52	ASN	2.8
1	2-A	52	ASN	2.8
1	3-A	52	ASN	2.8
1	4-A	52	ASN	2.8
1	5-A	52	ASN	2.8
1	6-A	52	ASN	2.8
1	7-A	52	ASN	2.8
1	8-A	52	ASN	2.8
1	9-A	52	ASN	2.8
1	10-A	52	ASN	2.8
1	11-A	52	ASN	2.8
1	12-A	52	ASN	2.8
1	13-A	52	ASN	2.8
1	14-A	52	ASN	2.8
1	15-A	52	ASN	2.8
1	16-A	52	ASN	2.8
1	1-A	303	GLU	2.8
1	2-A	303	GLU	2.8
1	3-A	303	GLU	2.8
1	4-A	303	GLU	2.8
1	5-A	303	GLU	2.8
1	6-A	303	GLU	2.8
1	7-A	303	GLU	2.8
1	8-A	303	GLU	2.8
1	9-A	303	GLU	2.8
1	10-A	303	GLU	2.8
1	11-A	303	GLU	2.8
1	12-A	303	GLU	2.8
1	13-A	303	GLU	2.8
1	14-A	303	GLU	2.8
1	15-A	303	GLU	2.8
1	16-A	303	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-A	316	ARG	2.8
1	2-A	316	ARG	2.8
1	3-A	316	ARG	2.8
1	4-A	316	ARG	2.8
1	5-A	316	ARG	2.8
1	6-A	316	ARG	2.8
1	7-A	316	ARG	2.8
1	8-A	316	ARG	2.8
1	9-A	316	ARG	2.8
1	10-A	316	ARG	2.8
1	11-A	316	ARG	2.8
1	12-A	316	ARG	2.8
1	13-A	316	ARG	2.8
1	14-A	316	ARG	2.8
1	15-A	316	ARG	2.8
1	16-A	316	ARG	2.8
1	1-A	302	THR	2.8
1	2-A	302	THR	2.8
1	3-A	302	THR	2.8
1	4-A	302	THR	2.8
1	5-A	302	THR	2.8
1	6-A	302	THR	2.8
1	7-A	302	THR	2.8
1	8-A	302	THR	2.8
1	9-A	302	THR	2.8
1	10-A	302	THR	2.8
1	11-A	302	THR	2.8
1	12-A	302	THR	2.8
1	13-A	302	THR	2.8
1	14-A	302	THR	2.8
1	15-A	302	THR	2.8
1	16-A	302	THR	2.8
1	1-A	108	VAL	2.8
1	2-A	108	VAL	2.8
1	3-A	108	VAL	2.8
1	4-A	108	VAL	2.8
1	5-A	108	VAL	2.8
1	6-A	108	VAL	2.8
1	7-A	108	VAL	2.8
1	8-A	108	VAL	2.8
1	9-A	108	VAL	2.8
1	10-A	108	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	11-A	108	VAL	2.8
1	12-A	108	VAL	2.8
1	13-A	108	VAL	2.8
1	14-A	108	VAL	2.8
1	15-A	108	VAL	2.8
1	16-A	108	VAL	2.8
1	1-A	204	LEU	2.7
1	2-A	204	LEU	2.7
1	3-A	204	LEU	2.7
1	4-A	204	LEU	2.7
1	5-A	204	LEU	2.7
1	6-A	204	LEU	2.7
1	7-A	204	LEU	2.7
1	8-A	204	LEU	2.7
1	9-A	204	LEU	2.7
1	10-A	204	LEU	2.7
1	11-A	204	LEU	2.7
1	12-A	204	LEU	2.7
1	13-A	204	LEU	2.7
1	14-A	204	LEU	2.7
1	15-A	204	LEU	2.7
1	16-A	204	LEU	2.7
1	1-B	323	ASN	2.7
1	2-B	323	ASN	2.7
1	3-B	323	ASN	2.7
1	4-B	323	ASN	2.7
1	5-B	323	ASN	2.7
1	6-B	323	ASN	2.7
1	7-B	323	ASN	2.7
1	8-B	323	ASN	2.7
1	9-B	323	ASN	2.7
1	10-B	323	ASN	2.7
1	11-B	323	ASN	2.7
1	12-B	323	ASN	2.7
1	13-B	323	ASN	2.7
1	14-B	323	ASN	2.7
1	15-B	323	ASN	2.7
1	16-B	323	ASN	2.7
1	1-B	71	GLU	2.7
1	2-B	71	GLU	2.7
1	3-B	71	GLU	2.7
1	4-B	71	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	5-B	71	GLU	2.7
1	6-B	71	GLU	2.7
1	7-B	71	GLU	2.7
1	8-B	71	GLU	2.7
1	9-B	71	GLU	2.7
1	10-B	71	GLU	2.7
1	11-B	71	GLU	2.7
1	12-B	71	GLU	2.7
1	13-B	71	GLU	2.7
1	14-B	71	GLU	2.7
1	15-B	71	GLU	2.7
1	16-B	71	GLU	2.7
1	1-A	282	ALA	2.7
1	2-A	282	ALA	2.7
1	3-A	282	ALA	2.7
1	4-A	282	ALA	2.7
1	5-A	282	ALA	2.7
1	6-A	282	ALA	2.7
1	7-A	282	ALA	2.7
1	8-A	282	ALA	2.7
1	9-A	282	ALA	2.7
1	10-A	282	ALA	2.7
1	11-A	282	ALA	2.7
1	12-A	282	ALA	2.7
1	13-A	282	ALA	2.7
1	14-A	282	ALA	2.7
1	15-A	282	ALA	2.7
1	16-A	282	ALA	2.7
1	1-A	6	GLN	2.6
1	2-A	6	GLN	2.6
1	3-A	6	GLN	2.6
1	4-A	6	GLN	2.6
1	5-A	6	GLN	2.6
1	6-A	6	GLN	2.6
1	7-A	6	GLN	2.6
1	8-A	6	GLN	2.6
1	9-A	6	GLN	2.6
1	10-A	6	GLN	2.6
1	11-A	6	GLN	2.6
1	12-A	6	GLN	2.6
1	13-A	6	GLN	2.6
1	14-A	6	GLN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	15-A	6	GLN	2.6
1	16-A	6	GLN	2.6
1	1-B	286	ASP	2.6
1	2-B	286	ASP	2.6
1	3-B	286	ASP	2.6
1	4-B	286	ASP	2.6
1	5-B	286	ASP	2.6
1	6-B	286	ASP	2.6
1	7-B	286	ASP	2.6
1	8-B	286	ASP	2.6
1	9-B	286	ASP	2.6
1	10-B	286	ASP	2.6
1	11-B	286	ASP	2.6
1	12-B	286	ASP	2.6
1	13-B	286	ASP	2.6
1	14-B	286	ASP	2.6
1	15-B	286	ASP	2.6
1	16-B	286	ASP	2.6
1	1-B	165	ASP	2.6
1	2-B	165	ASP	2.6
1	3-B	165	ASP	2.6
1	4-B	165	ASP	2.6
1	5-B	165	ASP	2.6
1	6-B	165	ASP	2.6
1	7-B	165	ASP	2.6
1	8-B	165	ASP	2.6
1	9-B	165	ASP	2.6
1	10-B	165	ASP	2.6
1	11-B	165	ASP	2.6
1	12-B	165	ASP	2.6
1	13-B	165	ASP	2.6
1	14-B	165	ASP	2.6
1	15-B	165	ASP	2.6
1	16-B	165	ASP	2.6
1	1-B	26	HIS	2.6
1	2-B	26	HIS	2.6
1	3-B	26	HIS	2.6
1	4-B	26	HIS	2.6
1	5-B	26	HIS	2.6
1	6-B	26	HIS	2.6
1	7-B	26	HIS	2.6
1	8-B	26	HIS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	9-B	26	HIS	2.6
1	10-B	26	HIS	2.6
1	11-B	26	HIS	2.6
1	12-B	26	HIS	2.6
1	13-B	26	HIS	2.6
1	14-B	26	HIS	2.6
1	15-B	26	HIS	2.6
1	16-B	26	HIS	2.6
1	1-A	272	THR	2.6
1	2-A	272	THR	2.6
1	3-A	272	THR	2.6
1	4-A	272	THR	2.6
1	5-A	272	THR	2.6
1	6-A	272	THR	2.6
1	7-A	272	THR	2.6
1	8-A	272	THR	2.6
1	9-A	272	THR	2.6
1	10-A	272	THR	2.6
1	11-A	272	THR	2.6
1	12-A	272	THR	2.6
1	13-A	272	THR	2.6
1	14-A	272	THR	2.6
1	15-A	272	THR	2.6
1	16-A	272	THR	2.6
1	1-A	38	SER	2.6
1	2-A	38	SER	2.6
1	3-A	38	SER	2.6
1	4-A	38	SER	2.6
1	5-A	38	SER	2.6
1	6-A	38	SER	2.6
1	7-A	38	SER	2.6
1	8-A	38	SER	2.6
1	9-A	38	SER	2.6
1	10-A	38	SER	2.6
1	11-A	38	SER	2.6
1	12-A	38	SER	2.6
1	13-A	38	SER	2.6
1	14-A	38	SER	2.6
1	15-A	38	SER	2.6
1	16-A	38	SER	2.6
1	1-A	301	LYS	2.5
1	2-A	301	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	3-A	301	LYS	2.5
1	4-A	301	LYS	2.5
1	5-A	301	LYS	2.5
1	6-A	301	LYS	2.5
1	7-A	301	LYS	2.5
1	8-A	301	LYS	2.5
1	9-A	301	LYS	2.5
1	10-A	301	LYS	2.5
1	11-A	301	LYS	2.5
1	12-A	301	LYS	2.5
1	13-A	301	LYS	2.5
1	14-A	301	LYS	2.5
1	15-A	301	LYS	2.5
1	16-A	301	LYS	2.5
1	1-A	122	GLY	2.5
1	2-A	122	GLY	2.5
1	3-A	122	GLY	2.5
1	4-A	122	GLY	2.5
1	5-A	122	GLY	2.5
1	6-A	122	GLY	2.5
1	7-A	122	GLY	2.5
1	8-A	122	GLY	2.5
1	9-A	122	GLY	2.5
1	10-A	122	GLY	2.5
1	11-A	122	GLY	2.5
1	12-A	122	GLY	2.5
1	13-A	122	GLY	2.5
1	14-A	122	GLY	2.5
1	15-A	122	GLY	2.5
1	16-A	122	GLY	2.5
1	1-B	232	GLU	2.5
1	2-B	232	GLU	2.5
1	3-B	232	GLU	2.5
1	4-B	232	GLU	2.5
1	5-B	232	GLU	2.5
1	6-B	232	GLU	2.5
1	7-B	232	GLU	2.5
1	8-B	232	GLU	2.5
1	9-B	232	GLU	2.5
1	10-B	232	GLU	2.5
1	11-B	232	GLU	2.5
1	12-B	232	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	13-B	232	GLU	2.5
1	14-B	232	GLU	2.5
1	15-B	232	GLU	2.5
1	16-B	232	GLU	2.5
1	1-A	355	GLN	2.5
1	2-A	355	GLN	2.5
1	3-A	355	GLN	2.5
1	4-A	355	GLN	2.5
1	5-A	355	GLN	2.5
1	6-A	355	GLN	2.5
1	7-A	355	GLN	2.5
1	8-A	355	GLN	2.5
1	9-A	355	GLN	2.5
1	10-A	355	GLN	2.5
1	11-A	355	GLN	2.5
1	12-A	355	GLN	2.5
1	13-A	355	GLN	2.5
1	14-A	355	GLN	2.5
1	15-A	355	GLN	2.5
1	16-A	355	GLN	2.5
1	1-B	292	VAL	2.5
1	2-B	292	VAL	2.5
1	3-B	292	VAL	2.5
1	4-B	292	VAL	2.5
1	5-B	292	VAL	2.5
1	6-B	292	VAL	2.5
1	7-B	292	VAL	2.5
1	8-B	292	VAL	2.5
1	9-B	292	VAL	2.5
1	10-B	292	VAL	2.5
1	11-B	292	VAL	2.5
1	12-B	292	VAL	2.5
1	13-B	292	VAL	2.5
1	14-B	292	VAL	2.5
1	15-B	292	VAL	2.5
1	16-B	292	VAL	2.5
1	1-A	7	ILE	2.4
1	2-A	7	ILE	2.4
1	3-A	7	ILE	2.4
1	4-A	7	ILE	2.4
1	5-A	7	ILE	2.4
1	6-A	7	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	7-A	7	ILE	2.4
1	8-A	7	ILE	2.4
1	9-A	7	ILE	2.4
1	10-A	7	ILE	2.4
1	11-A	7	ILE	2.4
1	12-A	7	ILE	2.4
1	13-A	7	ILE	2.4
1	14-A	7	ILE	2.4
1	15-A	7	ILE	2.4
1	16-A	7	ILE	2.4
1	1-A	166	GLU	2.4
1	2-A	166	GLU	2.4
1	3-A	166	GLU	2.4
1	4-A	166	GLU	2.4
1	5-A	166	GLU	2.4
1	6-A	166	GLU	2.4
1	7-A	166	GLU	2.4
1	8-A	166	GLU	2.4
1	9-A	166	GLU	2.4
1	10-A	166	GLU	2.4
1	11-A	166	GLU	2.4
1	12-A	166	GLU	2.4
1	13-A	166	GLU	2.4
1	14-A	166	GLU	2.4
1	15-A	166	GLU	2.4
1	16-A	166	GLU	2.4
1	1-A	230	SER	2.4
1	2-A	230	SER	2.4
1	3-A	230	SER	2.4
1	4-A	230	SER	2.4
1	5-A	230	SER	2.4
1	6-A	230	SER	2.4
1	7-A	230	SER	2.4
1	8-A	230	SER	2.4
1	9-A	230	SER	2.4
1	10-A	230	SER	2.4
1	11-A	230	SER	2.4
1	12-A	230	SER	2.4
1	13-A	230	SER	2.4
1	14-A	230	SER	2.4
1	15-A	230	SER	2.4
1	16-A	230	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-B	219	ALA	2.4
1	2-B	219	ALA	2.4
1	3-B	219	ALA	2.4
1	4-B	219	ALA	2.4
1	5-B	219	ALA	2.4
1	6-B	219	ALA	2.4
1	7-B	219	ALA	2.4
1	8-B	219	ALA	2.4
1	9-B	219	ALA	2.4
1	10-B	219	ALA	2.4
1	11-B	219	ALA	2.4
1	12-B	219	ALA	2.4
1	13-B	219	ALA	2.4
1	14-B	219	ALA	2.4
1	15-B	219	ALA	2.4
1	16-B	219	ALA	2.4
1	1-A	201	ASN	2.4
1	2-A	201	ASN	2.4
1	3-A	201	ASN	2.4
1	4-A	201	ASN	2.4
1	5-A	201	ASN	2.4
1	6-A	201	ASN	2.4
1	7-A	201	ASN	2.4
1	8-A	201	ASN	2.4
1	9-A	201	ASN	2.4
1	10-A	201	ASN	2.4
1	11-A	201	ASN	2.4
1	12-A	201	ASN	2.4
1	13-A	201	ASN	2.4
1	14-A	201	ASN	2.4
1	15-A	201	ASN	2.4
1	16-A	201	ASN	2.4
1	1-B	360	SER	2.4
1	2-B	360	SER	2.4
1	3-B	360	SER	2.4
1	4-B	360	SER	2.4
1	5-B	360	SER	2.4
1	6-B	360	SER	2.4
1	7-B	360	SER	2.4
1	8-B	360	SER	2.4
1	9-B	360	SER	2.4
1	10-B	360	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	11-B	360	SER	2.4
1	12-B	360	SER	2.4
1	13-B	360	SER	2.4
1	14-B	360	SER	2.4
1	15-B	360	SER	2.4
1	16-B	360	SER	2.4
1	1-A	24	ALA	2.4
1	2-A	24	ALA	2.4
1	3-A	24	ALA	2.4
1	4-A	24	ALA	2.4
1	5-A	24	ALA	2.4
1	6-A	24	ALA	2.4
1	7-A	24	ALA	2.4
1	8-A	24	ALA	2.4
1	9-A	24	ALA	2.4
1	10-A	24	ALA	2.4
1	11-A	24	ALA	2.4
1	12-A	24	ALA	2.4
1	13-A	24	ALA	2.4
1	14-A	24	ALA	2.4
1	15-A	24	ALA	2.4
1	16-A	24	ALA	2.4
1	1-B	216	LEU	2.4
1	2-B	216	LEU	2.4
1	3-B	216	LEU	2.4
1	4-B	216	LEU	2.4
1	5-B	216	LEU	2.4
1	6-B	216	LEU	2.4
1	7-B	216	LEU	2.4
1	8-B	216	LEU	2.4
1	9-B	216	LEU	2.4
1	10-B	216	LEU	2.4
1	11-B	216	LEU	2.4
1	12-B	216	LEU	2.4
1	13-B	216	LEU	2.4
1	14-B	216	LEU	2.4
1	15-B	216	LEU	2.4
1	16-B	216	LEU	2.4
1	1-A	27	LEU	2.3
1	2-A	27	LEU	2.3
1	3-A	27	LEU	2.3
1	4-A	27	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	5-A	27	LEU	2.3
1	6-A	27	LEU	2.3
1	7-A	27	LEU	2.3
1	8-A	27	LEU	2.3
1	9-A	27	LEU	2.3
1	10-A	27	LEU	2.3
1	11-A	27	LEU	2.3
1	12-A	27	LEU	2.3
1	13-A	27	LEU	2.3
1	14-A	27	LEU	2.3
1	15-A	27	LEU	2.3
1	16-A	27	LEU	2.3
1	1-A	192	ALA	2.3
1	2-A	192	ALA	2.3
1	3-A	192	ALA	2.3
1	4-A	192	ALA	2.3
1	5-A	192	ALA	2.3
1	6-A	192	ALA	2.3
1	7-A	192	ALA	2.3
1	8-A	192	ALA	2.3
1	9-A	192	ALA	2.3
1	10-A	192	ALA	2.3
1	11-A	192	ALA	2.3
1	12-A	192	ALA	2.3
1	13-A	192	ALA	2.3
1	14-A	192	ALA	2.3
1	15-A	192	ALA	2.3
1	16-A	192	ALA	2.3
1	1-A	41	LEU	2.3
1	1-A	334	SER	2.3
1	2-A	41	LEU	2.3
1	2-A	334	SER	2.3
1	3-A	41	LEU	2.3
1	3-A	334	SER	2.3
1	4-A	41	LEU	2.3
1	4-A	334	SER	2.3
1	5-A	41	LEU	2.3
1	5-A	334	SER	2.3
1	6-A	41	LEU	2.3
1	6-A	334	SER	2.3
1	7-A	41	LEU	2.3
1	7-A	334	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	8-A	41	LEU	2.3
1	8-A	334	SER	2.3
1	9-A	41	LEU	2.3
1	9-A	334	SER	2.3
1	10-A	41	LEU	2.3
1	10-A	334	SER	2.3
1	11-A	41	LEU	2.3
1	11-A	334	SER	2.3
1	12-A	41	LEU	2.3
1	12-A	334	SER	2.3
1	13-A	41	LEU	2.3
1	13-A	334	SER	2.3
1	14-A	41	LEU	2.3
1	14-A	334	SER	2.3
1	15-A	41	LEU	2.3
1	15-A	334	SER	2.3
1	16-A	41	LEU	2.3
1	16-A	334	SER	2.3
1	1-B	350	VAL	2.3
1	2-B	350	VAL	2.3
1	3-B	350	VAL	2.3
1	4-B	350	VAL	2.3
1	5-B	350	VAL	2.3
1	6-B	350	VAL	2.3
1	7-B	350	VAL	2.3
1	8-B	350	VAL	2.3
1	9-B	350	VAL	2.3
1	10-B	350	VAL	2.3
1	11-B	350	VAL	2.3
1	12-B	350	VAL	2.3
1	13-B	350	VAL	2.3
1	14-B	350	VAL	2.3
1	15-B	350	VAL	2.3
1	16-B	350	VAL	2.3
1	1-A	95	GLY	2.3
1	2-A	95	GLY	2.3
1	3-A	95	GLY	2.3
1	4-A	95	GLY	2.3
1	5-A	95	GLY	2.3
1	6-A	95	GLY	2.3
1	7-A	95	GLY	2.3
1	8-A	95	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	9-A	95	GLY	2.3
1	10-A	95	GLY	2.3
1	11-A	95	GLY	2.3
1	12-A	95	GLY	2.3
1	13-A	95	GLY	2.3
1	14-A	95	GLY	2.3
1	15-A	95	GLY	2.3
1	16-A	95	GLY	2.3
1	1-B	218	GLU	2.3
1	2-B	218	GLU	2.3
1	3-B	218	GLU	2.3
1	4-B	218	GLU	2.3
1	5-B	218	GLU	2.3
1	6-B	218	GLU	2.3
1	7-B	218	GLU	2.3
1	8-B	218	GLU	2.3
1	9-B	218	GLU	2.3
1	10-B	218	GLU	2.3
1	11-B	218	GLU	2.3
1	12-B	218	GLU	2.3
1	13-B	218	GLU	2.3
1	14-B	218	GLU	2.3
1	15-B	218	GLU	2.3
1	16-B	218	GLU	2.3
1	1-A	168	PHE	2.3
1	1-A	202	PHE	2.3
1	2-A	168	PHE	2.3
1	2-A	202	PHE	2.3
1	3-A	168	PHE	2.3
1	3-A	202	PHE	2.3
1	4-A	168	PHE	2.3
1	4-A	202	PHE	2.3
1	5-A	168	PHE	2.3
1	5-A	202	PHE	2.3
1	6-A	168	PHE	2.3
1	6-A	202	PHE	2.3
1	7-A	168	PHE	2.3
1	7-A	202	PHE	2.3
1	8-A	168	PHE	2.3
1	8-A	202	PHE	2.3
1	9-A	168	PHE	2.3
1	9-A	202	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	10-A	168	PHE	2.3
1	10-A	202	PHE	2.3
1	11-A	168	PHE	2.3
1	11-A	202	PHE	2.3
1	12-A	168	PHE	2.3
1	12-A	202	PHE	2.3
1	13-A	168	PHE	2.3
1	13-A	202	PHE	2.3
1	14-A	168	PHE	2.3
1	14-A	202	PHE	2.3
1	15-A	168	PHE	2.3
1	15-A	202	PHE	2.3
1	16-A	168	PHE	2.3
1	16-A	202	PHE	2.3
1	1-B	304	LEU	2.2
1	2-B	304	LEU	2.2
1	3-B	304	LEU	2.2
1	4-B	304	LEU	2.2
1	5-B	304	LEU	2.2
1	6-B	304	LEU	2.2
1	7-B	304	LEU	2.2
1	8-B	304	LEU	2.2
1	9-B	304	LEU	2.2
1	10-B	304	LEU	2.2
1	11-B	304	LEU	2.2
1	12-B	304	LEU	2.2
1	13-B	304	LEU	2.2
1	14-B	304	LEU	2.2
1	15-B	304	LEU	2.2
1	16-B	304	LEU	2.2
1	1-B	331	TYR	2.2
1	2-B	331	TYR	2.2
1	3-B	331	TYR	2.2
1	4-B	331	TYR	2.2
1	5-B	331	TYR	2.2
1	6-B	331	TYR	2.2
1	7-B	331	TYR	2.2
1	8-B	331	TYR	2.2
1	9-B	331	TYR	2.2
1	10-B	331	TYR	2.2
1	11-B	331	TYR	2.2
1	12-B	331	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	13-B	331	TYR	2.2
1	14-B	331	TYR	2.2
1	15-B	331	TYR	2.2
1	16-B	331	TYR	2.2
1	1-B	152	GLN	2.2
1	2-B	152	GLN	2.2
1	3-B	152	GLN	2.2
1	4-B	152	GLN	2.2
1	5-B	152	GLN	2.2
1	6-B	152	GLN	2.2
1	7-B	152	GLN	2.2
1	8-B	152	GLN	2.2
1	9-B	152	GLN	2.2
1	10-B	152	GLN	2.2
1	11-B	152	GLN	2.2
1	12-B	152	GLN	2.2
1	13-B	152	GLN	2.2
1	14-B	152	GLN	2.2
1	15-B	152	GLN	2.2
1	16-B	152	GLN	2.2
1	1-A	312	ARG	2.2
1	2-A	312	ARG	2.2
1	3-A	312	ARG	2.2
1	4-A	312	ARG	2.2
1	5-A	312	ARG	2.2
1	6-A	312	ARG	2.2
1	7-A	312	ARG	2.2
1	8-A	312	ARG	2.2
1	9-A	312	ARG	2.2
1	10-A	312	ARG	2.2
1	11-A	312	ARG	2.2
1	12-A	312	ARG	2.2
1	13-A	312	ARG	2.2
1	14-A	312	ARG	2.2
1	15-A	312	ARG	2.2
1	16-A	312	ARG	2.2
1	1-B	43	LYS	2.2
1	2-B	43	LYS	2.2
1	3-B	43	LYS	2.2
1	4-B	43	LYS	2.2
1	5-B	43	LYS	2.2
1	6-B	43	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	7-B	43	LYS	2.2
1	8-B	43	LYS	2.2
1	9-B	43	LYS	2.2
1	10-B	43	LYS	2.2
1	11-B	43	LYS	2.2
1	12-B	43	LYS	2.2
1	13-B	43	LYS	2.2
1	14-B	43	LYS	2.2
1	15-B	43	LYS	2.2
1	16-B	43	LYS	2.2
1	1-A	53	TYR	2.1
1	2-A	53	TYR	2.1
1	3-A	53	TYR	2.1
1	4-A	53	TYR	2.1
1	5-A	53	TYR	2.1
1	6-A	53	TYR	2.1
1	7-A	53	TYR	2.1
1	8-A	53	TYR	2.1
1	9-A	53	TYR	2.1
1	10-A	53	TYR	2.1
1	11-A	53	TYR	2.1
1	12-A	53	TYR	2.1
1	13-A	53	TYR	2.1
1	14-A	53	TYR	2.1
1	15-A	53	TYR	2.1
1	16-A	53	TYR	2.1
1	1-B	203	GLU	2.1
1	2-B	203	GLU	2.1
1	3-B	203	GLU	2.1
1	4-B	203	GLU	2.1
1	5-B	203	GLU	2.1
1	6-B	203	GLU	2.1
1	7-B	203	GLU	2.1
1	8-B	203	GLU	2.1
1	9-B	203	GLU	2.1
1	10-B	203	GLU	2.1
1	11-B	203	GLU	2.1
1	12-B	203	GLU	2.1
1	13-B	203	GLU	2.1
1	14-B	203	GLU	2.1
1	15-B	203	GLU	2.1
1	16-B	203	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-B	230	SER	2.1
1	2-B	230	SER	2.1
1	3-B	230	SER	2.1
1	4-B	230	SER	2.1
1	5-B	230	SER	2.1
1	6-B	230	SER	2.1
1	7-B	230	SER	2.1
1	8-B	230	SER	2.1
1	9-B	230	SER	2.1
1	10-B	230	SER	2.1
1	11-B	230	SER	2.1
1	12-B	230	SER	2.1
1	13-B	230	SER	2.1
1	14-B	230	SER	2.1
1	15-B	230	SER	2.1
1	16-B	230	SER	2.1
1	1-A	203	GLU	2.1
1	2-A	203	GLU	2.1
1	3-A	203	GLU	2.1
1	4-A	203	GLU	2.1
1	5-A	203	GLU	2.1
1	6-A	203	GLU	2.1
1	7-A	203	GLU	2.1
1	8-A	203	GLU	2.1
1	9-A	203	GLU	2.1
1	10-A	203	GLU	2.1
1	11-A	203	GLU	2.1
1	12-A	203	GLU	2.1
1	13-A	203	GLU	2.1
1	14-A	203	GLU	2.1
1	15-A	203	GLU	2.1
1	16-A	203	GLU	2.1
1	1-B	37	ALA	2.1
1	2-B	37	ALA	2.1
1	3-B	37	ALA	2.1
1	4-B	37	ALA	2.1
1	5-B	37	ALA	2.1
1	6-B	37	ALA	2.1
1	7-B	37	ALA	2.1
1	8-B	37	ALA	2.1
1	9-B	37	ALA	2.1
1	10-B	37	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	11-B	37	ALA	2.1
1	12-B	37	ALA	2.1
1	13-B	37	ALA	2.1
1	14-B	37	ALA	2.1
1	15-B	37	ALA	2.1
1	16-B	37	ALA	2.1
1	1-B	15	ALA	2.1
1	2-B	15	ALA	2.1
1	3-B	15	ALA	2.1
1	4-B	15	ALA	2.1
1	5-B	15	ALA	2.1
1	6-B	15	ALA	2.1
1	7-B	15	ALA	2.1
1	8-B	15	ALA	2.1
1	9-B	15	ALA	2.1
1	10-B	15	ALA	2.1
1	11-B	15	ALA	2.1
1	12-B	15	ALA	2.1
1	13-B	15	ALA	2.1
1	14-B	15	ALA	2.1
1	15-B	15	ALA	2.1
1	16-B	15	ALA	2.1
1	1-A	142	GLU	2.1
1	2-A	142	GLU	2.1
1	3-A	142	GLU	2.1
1	4-A	142	GLU	2.1
1	5-A	142	GLU	2.1
1	6-A	142	GLU	2.1
1	7-A	142	GLU	2.1
1	8-A	142	GLU	2.1
1	9-A	142	GLU	2.1
1	10-A	142	GLU	2.1
1	11-A	142	GLU	2.1
1	12-A	142	GLU	2.1
1	13-A	142	GLU	2.1
1	14-A	142	GLU	2.1
1	15-A	142	GLU	2.1
1	16-A	142	GLU	2.1
1	1-A	99	LEU	2.1
1	1-A	352	LYS	2.1
1	2-A	99	LEU	2.1
1	2-A	352	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	3-A	99	LEU	2.1
1	3-A	352	LYS	2.1
1	4-A	99	LEU	2.1
1	4-A	352	LYS	2.1
1	5-A	99	LEU	2.1
1	5-A	352	LYS	2.1
1	6-A	99	LEU	2.1
1	6-A	352	LYS	2.1
1	7-A	99	LEU	2.1
1	7-A	352	LYS	2.1
1	8-A	99	LEU	2.1
1	8-A	352	LYS	2.1
1	9-A	99	LEU	2.1
1	9-A	352	LYS	2.1
1	10-A	99	LEU	2.1
1	10-A	352	LYS	2.1
1	11-A	99	LEU	2.1
1	11-A	352	LYS	2.1
1	12-A	99	LEU	2.1
1	12-A	352	LYS	2.1
1	13-A	99	LEU	2.1
1	13-A	352	LYS	2.1
1	14-A	99	LEU	2.1
1	14-A	352	LYS	2.1
1	15-A	99	LEU	2.1
1	15-A	352	LYS	2.1
1	16-A	99	LEU	2.1
1	16-A	352	LYS	2.1
1	1-A	147	SER	2.0
1	2-A	147	SER	2.0
1	3-A	147	SER	2.0
1	4-A	147	SER	2.0
1	5-A	147	SER	2.0
1	6-A	147	SER	2.0
1	7-A	147	SER	2.0
1	8-A	147	SER	2.0
1	9-A	147	SER	2.0
1	10-A	147	SER	2.0
1	11-A	147	SER	2.0
1	12-A	147	SER	2.0
1	13-A	147	SER	2.0
1	14-A	147	SER	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	15-A	147	SER	2.0
1	16-A	147	SER	2.0
1	1-A	296	SER	2.0
1	2-A	296	SER	2.0
1	3-A	296	SER	2.0
1	4-A	296	SER	2.0
1	5-A	296	SER	2.0
1	6-A	296	SER	2.0
1	7-A	296	SER	2.0
1	8-A	296	SER	2.0
1	9-A	296	SER	2.0
1	10-A	296	SER	2.0
1	11-A	296	SER	2.0
1	12-A	296	SER	2.0
1	13-A	296	SER	2.0
1	14-A	296	SER	2.0
1	15-A	296	SER	2.0
1	16-A	296	SER	2.0
1	1-B	108	VAL	2.0
1	2-B	108	VAL	2.0
1	3-B	108	VAL	2.0
1	4-B	108	VAL	2.0
1	5-B	108	VAL	2.0
1	6-B	108	VAL	2.0
1	7-B	108	VAL	2.0
1	8-B	108	VAL	2.0
1	9-B	108	VAL	2.0
1	10-B	108	VAL	2.0
1	11-B	108	VAL	2.0
1	12-B	108	VAL	2.0
1	13-B	108	VAL	2.0
1	14-B	108	VAL	2.0
1	15-B	108	VAL	2.0
1	16-B	108	VAL	2.0
1	1-B	356	GLN	2.0
1	2-B	356	GLN	2.0
1	3-B	356	GLN	2.0
1	4-B	356	GLN	2.0
1	5-B	356	GLN	2.0
1	6-B	356	GLN	2.0
1	7-B	356	GLN	2.0
1	8-B	356	GLN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	9-B	356	GLN	2.0
1	10-B	356	GLN	2.0
1	11-B	356	GLN	2.0
1	12-B	356	GLN	2.0
1	13-B	356	GLN	2.0
1	14-B	356	GLN	2.0
1	15-B	356	GLN	2.0
1	16-B	356	GLN	2.0
1	1-B	327	LYS	2.0
1	2-B	327	LYS	2.0
1	3-B	327	LYS	2.0
1	4-B	327	LYS	2.0
1	5-B	327	LYS	2.0
1	6-B	327	LYS	2.0
1	7-B	327	LYS	2.0
1	8-B	327	LYS	2.0
1	9-B	327	LYS	2.0
1	10-B	327	LYS	2.0
1	11-B	327	LYS	2.0
1	12-B	327	LYS	2.0
1	13-B	327	LYS	2.0
1	14-B	327	LYS	2.0
1	15-B	327	LYS	2.0
1	16-B	327	LYS	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.