



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:26 PM UTC

PDB ID : 2Q4J / pdb_00002q4j
Title : Ensemble refinement of the protein crystal structure of gene product from Arabidopsis thaliana At3g03250, a putative UDP-glucose pyrophosphorylase
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 : 1.86 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

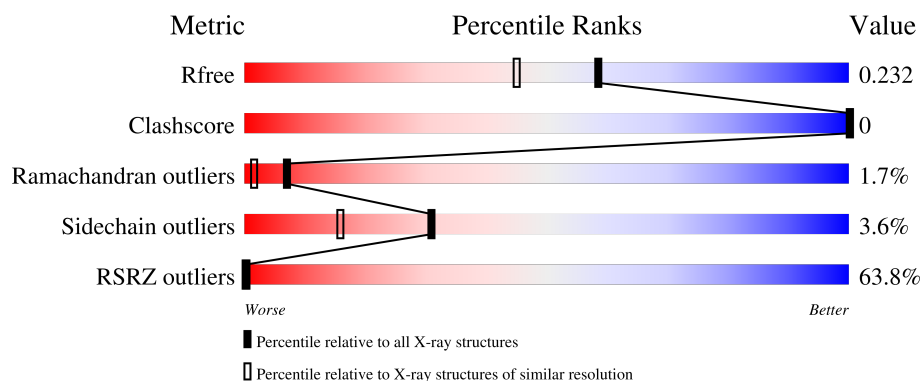
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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.



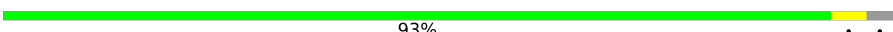
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	469	68% 93% 5% .
1	1-B	469	57% 93% . .
1	2-A	469	94% . .
1	2-B	469	93% . .
1	3-A	469	93% 5% .

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Mol	Chain	Length	Quality of chain
1	3-B	469	 93% • •
1	4-A	469	 92%6% •
1	4-B	469	 93% • •
1	5-A	469	 92%6% •
1	5-B	469	 93% • •
1	6-A	469	 93%5% •
1	6-B	469	 92%5% •
1	7-A	469	 93%5% •
1	7-B	469	 93% • •
1	8-A	469	 93%5% •
1	8-B	469	 93% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 60344 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 UTP-glucose-1-phosphate uridylyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	460	Total	C	N	O	S	0	0	0
			3579	2291	591	687	10			
1	2-A	460	Total	C	N	O	S	0	0	0
			3579	2291	591	687	10			
1	3-A	460	Total	C	N	O	S	0	0	0
			3579	2291	591	687	10			
1	4-A	460	Total	C	N	O	S	0	0	0
			3579	2291	591	687	10			
1	5-A	460	Total	C	N	O	S	0	0	0
			3579	2291	591	687	10			
1	6-A	460	Total	C	N	O	S	0	0	0
			3579	2291	591	687	10			
1	7-A	460	Total	C	N	O	S	0	0	0
			3579	2291	591	687	10			
1	8-A	460	Total	C	N	O	S	0	0	0
			3579	2291	591	687	10			
1	1-B	455	Total	C	N	O	S	0	0	0
			3543	2271	585	677	10			
1	2-B	455	Total	C	N	O	S	0	0	0
			3543	2271	585	677	10			
1	3-B	455	Total	C	N	O	S	0	0	0
			3543	2271	585	677	10			
1	4-B	455	Total	C	N	O	S	0	0	0
			3543	2271	585	677	10			
1	5-B	455	Total	C	N	O	S	0	0	0
			3543	2271	585	677	10			
1	6-B	455	Total	C	N	O	S	0	0	0
			3543	2271	585	677	10			
1	7-B	455	Total	C	N	O	S	0	0	0
			3543	2271	585	677	10			
1	8-B	455	Total	C	N	O	S	0	0	0
			3543	2271	585	677	10			

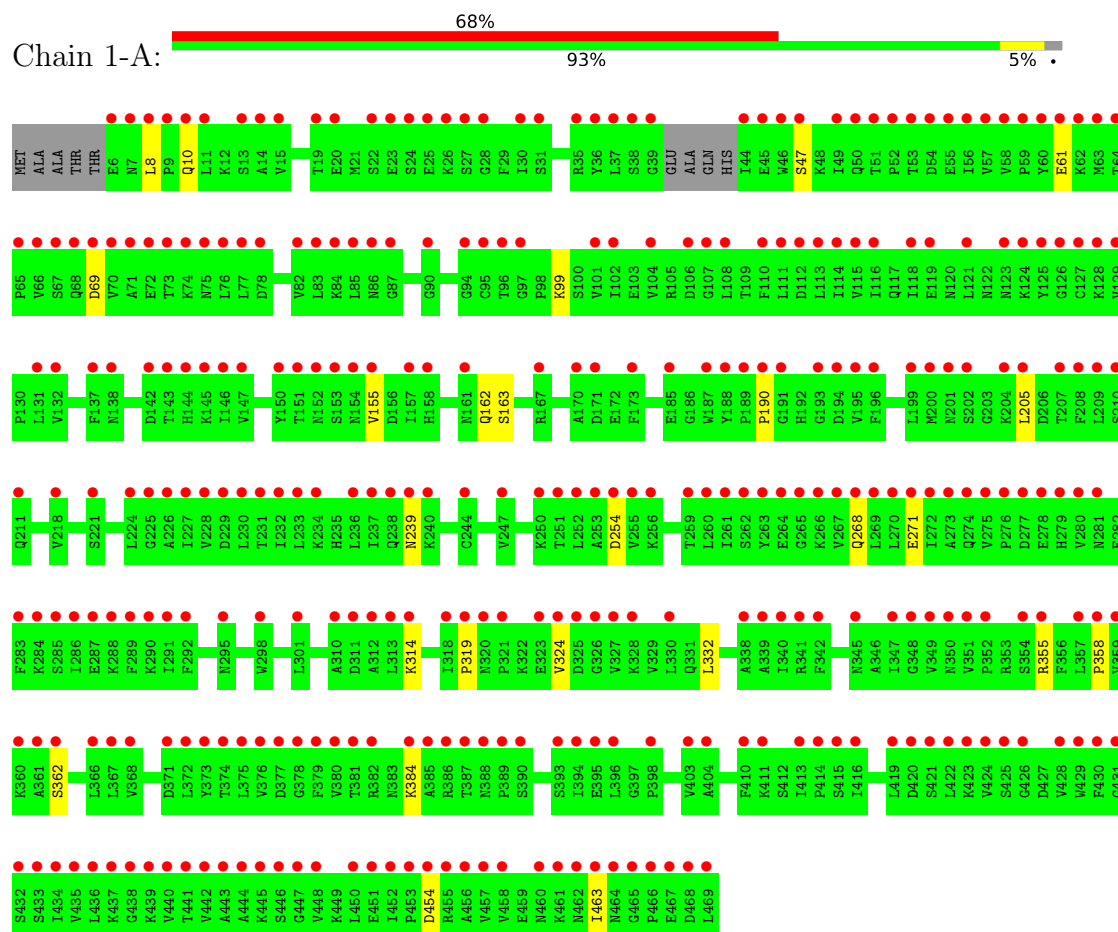
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1-A	180	Total 180	O 180	0	0
2	2-A	182	Total 182	O 182	0	0
2	3-A	182	Total 182	O 182	0	0
2	4-A	183	Total 183	O 183	0	0
2	5-A	182	Total 182	O 182	0	0
2	6-A	182	Total 182	O 182	0	0
2	7-A	183	Total 183	O 183	0	0
2	8-A	183	Total 183	O 183	0	0
2	1-B	241	Total 241	O 241	0	0
2	2-B	239	Total 239	O 239	0	0
2	3-B	239	Total 239	O 239	0	0
2	4-B	238	Total 238	O 238	0	0
2	5-B	239	Total 239	O 239	0	0
2	6-B	239	Total 239	O 239	0	0
2	7-B	238	Total 238	O 238	0	0
2	8-B	238	Total 238	O 238	0	0

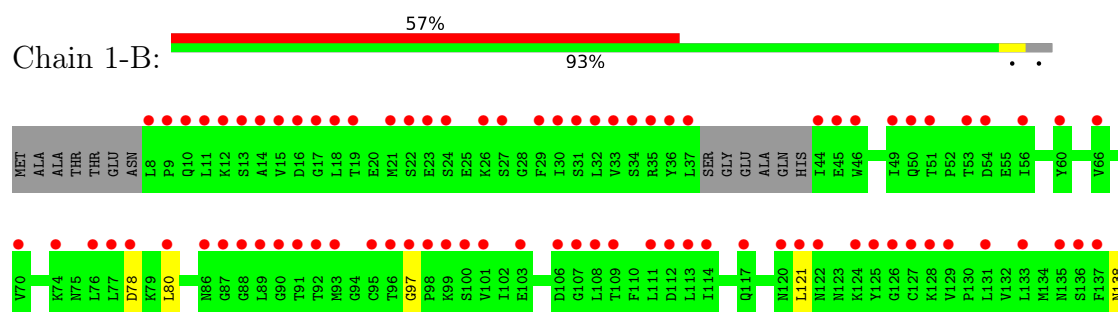
3 Residue-property plots [i](#)

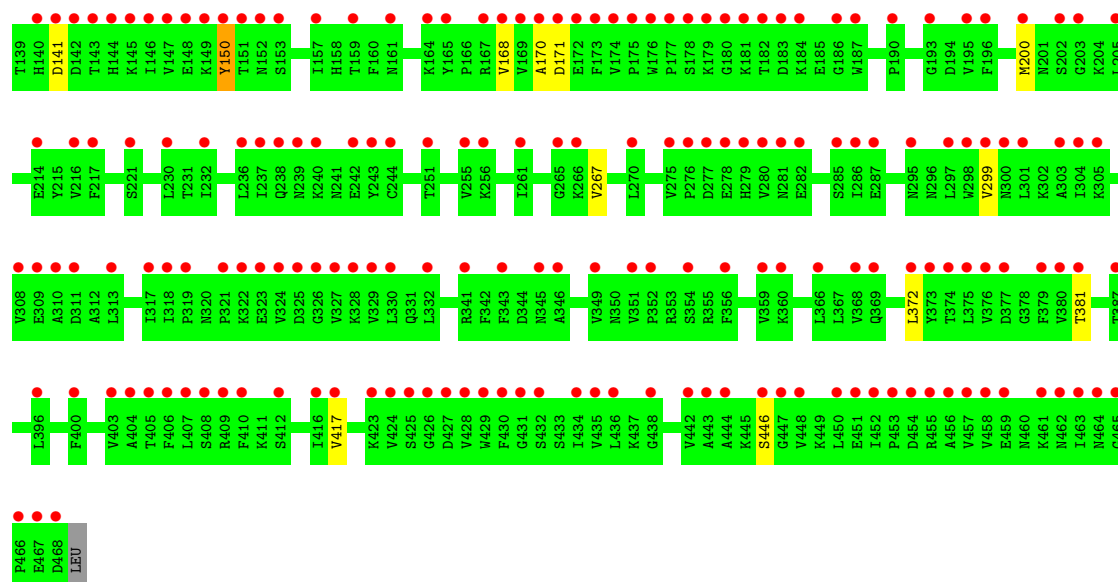
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2



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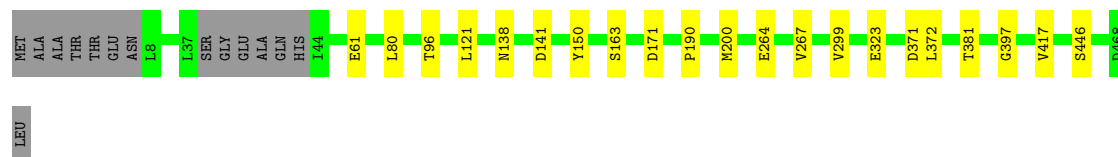
- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2

Chain 2-A: 94%



- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2

Chain 2-B: 93%



- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2

Chain 3-A: 93% 5%

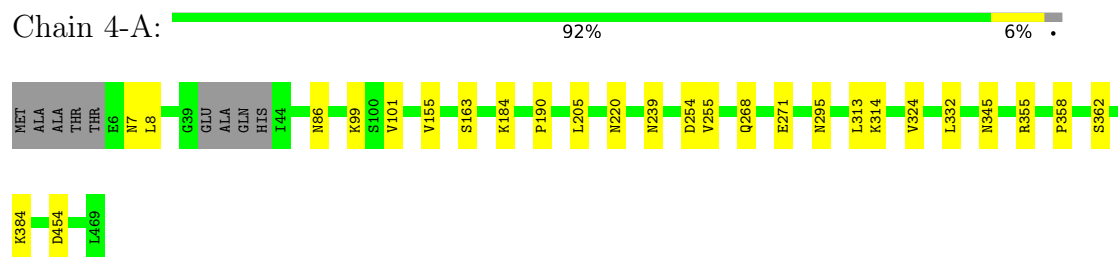


- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2

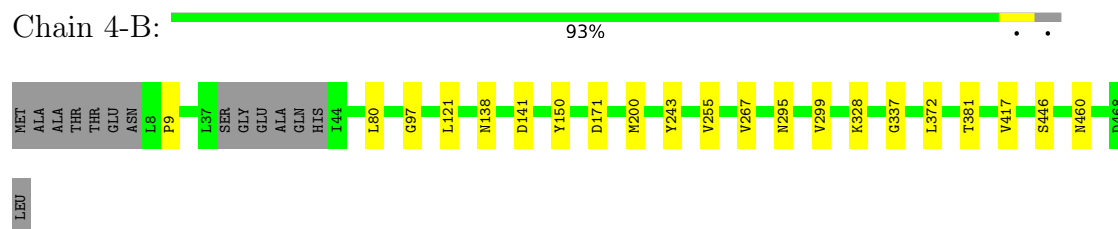
Chain 3-B: 93%



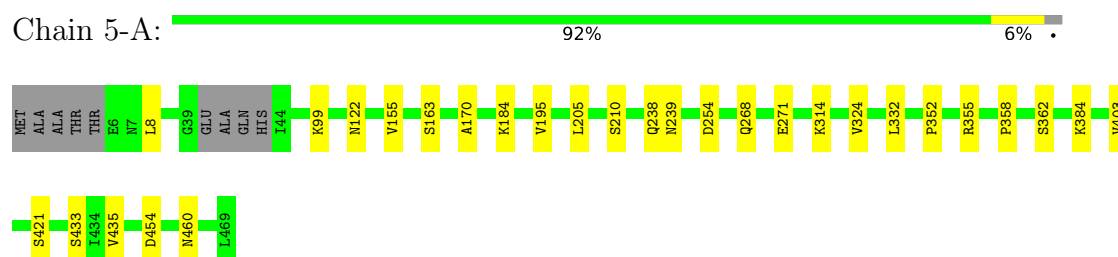
- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2



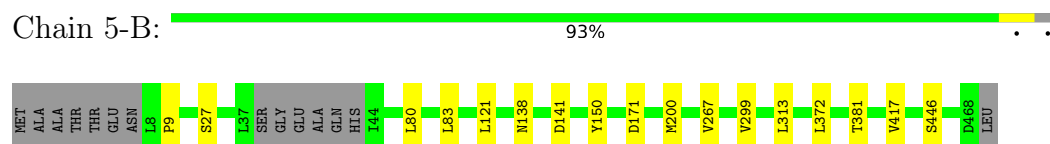
- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2



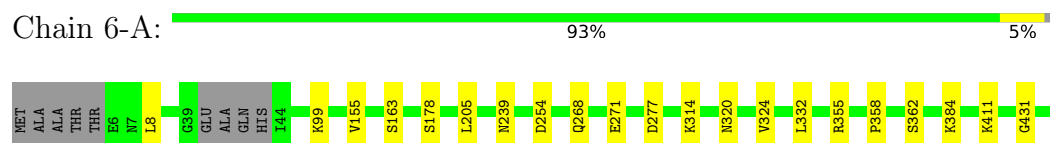
- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2



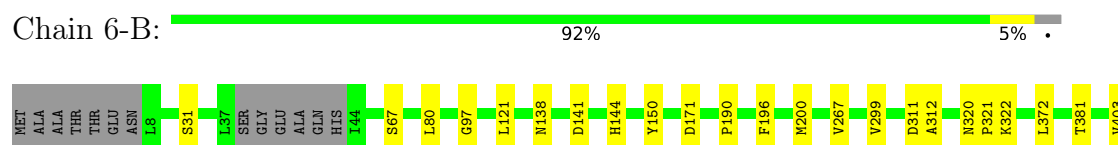
- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2



- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2



- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2





- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2

Chain 7-A: 93% 5% .



- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2

Chain 7-B: 93% . .



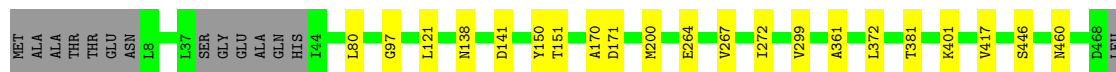
- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2

Chain 8-A: 93% 5% .



- Molecule 1: Probable UTP-glucose-1-phosphate uridylyltransferase 2

Chain 8-B: 93% . .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.68Å 58.86Å 89.86Å 90.00° 100.40° 90.00°	Depositor
Resolution (Å)	37.37 – 1.86 37.37 – 1.86	Depositor EDS
% Data completeness (in resolution range)	97.6 (37.37-1.86) 97.7 (37.37-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 1.87Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.171 , 0.231 0.174 , 0.232	Depositor DCC
R_{free} test set	3986 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.04 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	60344	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.24	0/3646	0.39	0/4942
1	1-B	0.25	0/3610	0.36	0/4895
1	2-A	0.24	0/3646	0.39	0/4942
1	2-B	0.25	0/3610	0.36	0/4895
1	3-A	0.24	0/3646	0.39	0/4942
1	3-B	0.25	0/3610	0.36	0/4895
1	4-A	0.24	0/3646	0.39	0/4942
1	4-B	0.25	0/3610	0.36	0/4895
1	5-A	0.24	0/3646	0.39	0/4942
1	5-B	0.25	0/3610	0.36	0/4895
1	6-A	0.24	0/3646	0.39	0/4942
1	6-B	0.25	0/3610	0.36	0/4895
1	7-A	0.24	0/3646	0.39	0/4942
1	7-B	0.25	0/3610	0.36	0/4895
1	8-A	0.24	0/3646	0.39	0/4942
1	8-B	0.25	0/3610	0.36	0/4895
All	All	0.25	0/58048	0.37	0/78696

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	3-B	0	1
1	4-B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	3-B	125	TYR	Sidechain
1	4-B	243	TYR	Sidechain

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	3579	0	3652	0	0
1	1-B	3543	0	3621	0	0
1	2-A	3579	0	3652	0	0
1	2-B	3543	0	3621	0	0
1	3-A	3579	0	3652	0	0
1	3-B	3543	0	3621	0	0
1	4-A	3579	0	3652	0	0
1	4-B	3543	0	3621	0	0
1	5-A	3579	0	3652	0	0
1	5-B	3543	0	3621	0	0
1	6-A	3579	0	3652	0	0
1	6-B	3543	0	3621	0	0
1	7-A	3579	0	3652	0	0
1	7-B	3543	0	3621	0	0
1	8-A	3579	0	3652	0	0
1	8-B	3543	0	3621	0	0
2	1-A	180	0	0	0	0
2	1-B	241	0	0	0	0
2	2-A	182	0	0	0	0
2	2-B	239	0	0	0	0
2	3-A	182	0	0	0	0
2	3-B	239	0	0	0	0
2	4-A	183	0	0	0	0
2	4-B	238	0	0	0	0
2	5-A	182	0	0	0	0
2	5-B	239	0	0	0	0
2	6-A	182	0	0	0	0
2	6-B	239	0	0	0	0
2	7-A	183	0	0	0	0
2	7-B	238	0	0	0	0
2	8-A	183	0	0	0	0
2	8-B	238	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	60344	0	58184	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	456/469 (97%)	399 (88%)	48 (10%)	9 (2%)	6	1
1	1-B	451/469 (96%)	408 (90%)	38 (8%)	5 (1%)	11	3
1	2-A	456/469 (97%)	407 (89%)	44 (10%)	5 (1%)	11	3
1	2-B	451/469 (96%)	405 (90%)	38 (8%)	8 (2%)	6	1
1	3-A	456/469 (97%)	415 (91%)	33 (7%)	8 (2%)	6	1
1	3-B	451/469 (96%)	410 (91%)	34 (8%)	7 (2%)	7	2
1	4-A	456/469 (97%)	403 (88%)	42 (9%)	11 (2%)	4	1
1	4-B	451/469 (96%)	411 (91%)	33 (7%)	7 (2%)	7	2
1	5-A	456/469 (97%)	406 (89%)	37 (8%)	13 (3%)	3	0
1	5-B	451/469 (96%)	406 (90%)	41 (9%)	4 (1%)	14	4
1	6-A	456/469 (97%)	402 (88%)	48 (10%)	6 (1%)	9	2
1	6-B	451/469 (96%)	399 (88%)	40 (9%)	12 (3%)	4	0
1	7-A	456/469 (97%)	415 (91%)	34 (8%)	7 (2%)	8	2
1	7-B	451/469 (96%)	407 (90%)	38 (8%)	6 (1%)	9	2
1	8-A	456/469 (97%)	403 (88%)	46 (10%)	7 (2%)	8	2
1	8-B	451/469 (96%)	409 (91%)	34 (8%)	8 (2%)	6	1
All	All	7256/7504 (97%)	6505 (90%)	628 (9%)	123 (2%)	7	1

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	8	LEU
1	1-B	170	ALA
1	3-A	38	SER
1	3-A	319	PRO
1	3-B	96	THR
1	3-B	97	GLY
1	4-A	8	LEU
1	4-A	220	ASN
1	4-B	255	VAL
1	4-B	295	ASN
1	4-B	460	ASN
1	5-A	403	VAL
1	5-A	433	SER
1	6-B	67	SER
1	6-B	311	ASP
1	6-B	321	PRO
1	6-B	322	LYS
1	7-A	38	SER
1	7-B	266	LYS
1	8-A	8	LEU
1	8-B	170	ALA
1	8-B	264	GLU
1	1-B	78	ASP
1	2-A	170	ALA
1	2-B	96	THR
1	2-B	264	GLU
1	2-B	323	GLU
1	3-A	387	THR
1	3-B	178	SER
1	4-A	313	LEU
1	5-A	460	ASN
1	5-B	9	PRO
1	5-B	27	SER
1	5-B	313	LEU
1	6-A	277	ASP
1	6-A	431	GLY
1	6-B	31	SER
1	6-B	97	GLY
1	6-B	403	VAL
1	7-A	8	LEU
1	7-A	202	SER
1	7-A	445	LYS

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Mol	Chain	Res	Type
1	7-A	460	ASN
1	7-B	155	VAL
1	7-B	403	VAL
1	8-A	340	ILE
1	1-A	47	SER
1	1-A	69	ASP
1	1-B	150	TYR
1	2-A	8	LEU
1	2-A	18	LEU
1	2-A	171	ASP
1	3-B	10	GLN
1	4-A	86	ASN
1	4-B	97	GLY
1	5-A	8	LEU
1	5-A	122	ASN
1	5-A	170	ALA
1	5-A	184	LYS
1	5-A	238	GLN
1	5-A	435	VAL
1	6-A	178	SER
1	6-A	411	LYS
1	8-A	371	ASP
1	8-A	419	LEU
1	8-B	361	ALA
1	8-B	401	LYS
1	1-A	61	GLU
1	1-A	463	ILE
1	2-B	371	ASP
1	3-A	386	ARG
1	4-A	7	ASN
1	4-A	101	VAL
1	4-A	184	LYS
1	4-B	328	LYS
1	5-A	210	SER
1	5-B	83	LEU
1	6-A	320	ASN
1	6-B	144	HIS
1	6-B	190	PRO
1	6-B	312	ALA
1	6-B	320	ASN
1	7-A	399	GLU
1	7-B	255	VAL

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Mol	Chain	Res	Type
1	8-A	105	ARG
1	8-B	97	GLY
1	1-A	10	GLN
1	1-A	319	PRO
1	1-B	97	GLY
1	1-B	168	VAL
1	2-A	191	GLY
1	2-B	61	GLU
1	2-B	163	SER
1	3-A	184	LYS
1	3-B	390	SER
1	4-A	295	ASN
1	5-A	421	SER
1	8-A	160	PHE
1	8-B	151	THR
1	8-B	272	ILE
1	8-B	460	ASN
1	1-A	162	GLN
1	2-B	190	PRO
1	2-B	397	GLY
1	4-A	345	ASN
1	4-B	337	GLY
1	6-B	196	PHE
1	7-B	265	GLY
1	8-A	313	LEU
1	3-A	9	PRO
1	3-B	56	ILE
1	4-B	9	PRO
1	6-A	8	LEU
1	7-B	190	PRO
1	1-A	190	PRO
1	4-A	190	PRO
1	3-A	70	VAL
1	3-A	320	ASN
1	3-B	57	VAL
1	4-A	255	VAL
1	5-A	352	PRO
1	5-A	195	VAL
1	7-A	197	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	408/414 (99%)	392 (96%)	16 (4%)	28	13
1	1-B	404/414 (98%)	391 (97%)	13 (3%)	34	19
1	2-A	408/414 (99%)	392 (96%)	16 (4%)	28	13
1	2-B	404/414 (98%)	391 (97%)	13 (3%)	34	19
1	3-A	408/414 (99%)	392 (96%)	16 (4%)	28	13
1	3-B	404/414 (98%)	391 (97%)	13 (3%)	34	19
1	4-A	408/414 (99%)	392 (96%)	16 (4%)	28	13
1	4-B	404/414 (98%)	391 (97%)	13 (3%)	34	19
1	5-A	408/414 (99%)	392 (96%)	16 (4%)	28	13
1	5-B	404/414 (98%)	391 (97%)	13 (3%)	34	19
1	6-A	408/414 (99%)	392 (96%)	16 (4%)	28	13
1	6-B	404/414 (98%)	391 (97%)	13 (3%)	34	19
1	7-A	408/414 (99%)	392 (96%)	16 (4%)	28	13
1	7-B	404/414 (98%)	391 (97%)	13 (3%)	34	19
1	8-A	408/414 (99%)	392 (96%)	16 (4%)	28	13
1	8-B	404/414 (98%)	391 (97%)	13 (3%)	34	19
All	All	6496/6624 (98%)	6264 (96%)	232 (4%)	31	16

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	99	LYS
1	1-A	155	VAL
1	1-A	163	SER
1	1-A	205	LEU
1	1-A	239	ASN
1	1-A	254	ASP
1	1-A	268	GLN
1	1-A	271	GLU

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Mol	Chain	Res	Type
1	1-A	314	LYS
1	1-A	324	VAL
1	1-A	332	LEU
1	1-A	355	ARG
1	1-A	358	PRO
1	1-A	362	SER
1	1-A	384	LYS
1	1-A	454	ASP
1	1-B	80	LEU
1	1-B	121	LEU
1	1-B	138	ASN
1	1-B	141	ASP
1	1-B	150	TYR
1	1-B	171	ASP
1	1-B	200	MET
1	1-B	267	VAL
1	1-B	299	VAL
1	1-B	372	LEU
1	1-B	381	THR
1	1-B	417	VAL
1	1-B	446	SER
1	2-A	99	LYS
1	2-A	155	VAL
1	2-A	163	SER
1	2-A	205	LEU
1	2-A	239	ASN
1	2-A	254	ASP
1	2-A	268	GLN
1	2-A	271	GLU
1	2-A	314	LYS
1	2-A	324	VAL
1	2-A	332	LEU
1	2-A	355	ARG
1	2-A	358	PRO
1	2-A	362	SER
1	2-A	384	LYS
1	2-A	454	ASP
1	2-B	80	LEU
1	2-B	121	LEU
1	2-B	138	ASN
1	2-B	141	ASP
1	2-B	150	TYR

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Mol	Chain	Res	Type
1	2-B	171	ASP
1	2-B	200	MET
1	2-B	267	VAL
1	2-B	299	VAL
1	2-B	372	LEU
1	2-B	381	THR
1	2-B	417	VAL
1	2-B	446	SER
1	3-A	99	LYS
1	3-A	155	VAL
1	3-A	163	SER
1	3-A	205	LEU
1	3-A	239	ASN
1	3-A	254	ASP
1	3-A	268	GLN
1	3-A	271	GLU
1	3-A	314	LYS
1	3-A	324	VAL
1	3-A	332	LEU
1	3-A	355	ARG
1	3-A	358	PRO
1	3-A	362	SER
1	3-A	384	LYS
1	3-A	454	ASP
1	3-B	80	LEU
1	3-B	121	LEU
1	3-B	138	ASN
1	3-B	141	ASP
1	3-B	150	TYR
1	3-B	171	ASP
1	3-B	200	MET
1	3-B	267	VAL
1	3-B	299	VAL
1	3-B	372	LEU
1	3-B	381	THR
1	3-B	417	VAL
1	3-B	446	SER
1	4-A	99	LYS
1	4-A	155	VAL
1	4-A	163	SER
1	4-A	205	LEU
1	4-A	239	ASN

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Mol	Chain	Res	Type
1	4-A	254	ASP
1	4-A	268	GLN
1	4-A	271	GLU
1	4-A	314	LYS
1	4-A	324	VAL
1	4-A	332	LEU
1	4-A	355	ARG
1	4-A	358	PRO
1	4-A	362	SER
1	4-A	384	LYS
1	4-A	454	ASP
1	4-B	80	LEU
1	4-B	121	LEU
1	4-B	138	ASN
1	4-B	141	ASP
1	4-B	150	TYR
1	4-B	171	ASP
1	4-B	200	MET
1	4-B	267	VAL
1	4-B	299	VAL
1	4-B	372	LEU
1	4-B	381	THR
1	4-B	417	VAL
1	4-B	446	SER
1	5-A	99	LYS
1	5-A	155	VAL
1	5-A	163	SER
1	5-A	205	LEU
1	5-A	239	ASN
1	5-A	254	ASP
1	5-A	268	GLN
1	5-A	271	GLU
1	5-A	314	LYS
1	5-A	324	VAL
1	5-A	332	LEU
1	5-A	355	ARG
1	5-A	358	PRO
1	5-A	362	SER
1	5-A	384	LYS
1	5-A	454	ASP
1	5-B	80	LEU
1	5-B	121	LEU

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Mol	Chain	Res	Type
1	5-B	138	ASN
1	5-B	141	ASP
1	5-B	150	TYR
1	5-B	171	ASP
1	5-B	200	MET
1	5-B	267	VAL
1	5-B	299	VAL
1	5-B	372	LEU
1	5-B	381	THR
1	5-B	417	VAL
1	5-B	446	SER
1	6-A	99	LYS
1	6-A	155	VAL
1	6-A	163	SER
1	6-A	205	LEU
1	6-A	239	ASN
1	6-A	254	ASP
1	6-A	268	GLN
1	6-A	271	GLU
1	6-A	314	LYS
1	6-A	324	VAL
1	6-A	332	LEU
1	6-A	355	ARG
1	6-A	358	PRO
1	6-A	362	SER
1	6-A	384	LYS
1	6-A	454	ASP
1	6-B	80	LEU
1	6-B	121	LEU
1	6-B	138	ASN
1	6-B	141	ASP
1	6-B	150	TYR
1	6-B	171	ASP
1	6-B	200	MET
1	6-B	267	VAL
1	6-B	299	VAL
1	6-B	372	LEU
1	6-B	381	THR
1	6-B	417	VAL
1	6-B	446	SER
1	7-A	99	LYS
1	7-A	155	VAL

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Mol	Chain	Res	Type
1	7-A	163	SER
1	7-A	205	LEU
1	7-A	239	ASN
1	7-A	254	ASP
1	7-A	268	GLN
1	7-A	271	GLU
1	7-A	314	LYS
1	7-A	324	VAL
1	7-A	332	LEU
1	7-A	355	ARG
1	7-A	358	PRO
1	7-A	362	SER
1	7-A	384	LYS
1	7-A	454	ASP
1	7-B	80	LEU
1	7-B	121	LEU
1	7-B	138	ASN
1	7-B	141	ASP
1	7-B	150	TYR
1	7-B	171	ASP
1	7-B	200	MET
1	7-B	267	VAL
1	7-B	299	VAL
1	7-B	372	LEU
1	7-B	381	THR
1	7-B	417	VAL
1	7-B	446	SER
1	8-A	99	LYS
1	8-A	155	VAL
1	8-A	163	SER
1	8-A	205	LEU
1	8-A	239	ASN
1	8-A	254	ASP
1	8-A	268	GLN
1	8-A	271	GLU
1	8-A	314	LYS
1	8-A	324	VAL
1	8-A	332	LEU
1	8-A	355	ARG
1	8-A	358	PRO
1	8-A	362	SER
1	8-A	384	LYS

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Mol	Chain	Res	Type
1	8-A	454	ASP
1	8-B	80	LEU
1	8-B	121	LEU
1	8-B	138	ASN
1	8-B	141	ASP
1	8-B	150	TYR
1	8-B	171	ASP
1	8-B	200	MET
1	8-B	267	VAL
1	8-B	299	VAL
1	8-B	372	LEU
1	8-B	381	THR
1	8-B	417	VAL
1	8-B	446	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	50	GLN
1	1-A	138	ASN
1	1-A	162	GLN
1	1-A	345	ASN
1	1-A	464	ASN
1	1-B	75	ASN
1	1-B	86	ASN
1	1-B	120	ASN
1	1-B	135	ASN
1	1-B	138	ASN
1	1-B	152	ASN
1	1-B	162	GLN
1	1-B	220	ASN
1	1-B	268	GLN
1	1-B	274	GLN
1	1-B	464	ASN
1	2-A	50	GLN
1	2-A	138	ASN
1	2-A	158	HIS
1	2-A	162	GLN
1	2-A	238	GLN
1	2-A	241	ASN
1	2-A	268	GLN
1	2-A	279	HIS

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Mol	Chain	Res	Type
1	2-A	391	ASN
1	2-B	50	GLN
1	2-B	138	ASN
1	2-B	152	ASN
1	2-B	162	GLN
1	2-B	192	HIS
1	2-B	220	ASN
1	2-B	235	HIS
1	2-B	239	ASN
1	2-B	279	HIS
1	2-B	295	ASN
1	2-B	345	ASN
1	3-A	10	GLN
1	3-A	50	GLN
1	3-A	68	GLN
1	3-A	75	ASN
1	3-A	158	HIS
1	3-A	235	HIS
1	3-A	268	GLN
1	3-A	296	ASN
1	3-A	345	ASN
1	3-A	460	ASN
1	3-B	10	GLN
1	3-B	50	GLN
1	3-B	75	ASN
1	3-B	120	ASN
1	3-B	138	ASN
1	3-B	152	ASN
1	3-B	162	GLN
1	3-B	220	ASN
1	3-B	268	GLN
1	3-B	279	HIS
1	3-B	293	ASN
1	3-B	295	ASN
1	4-A	68	GLN
1	4-A	75	ASN
1	4-A	117	GLN
1	4-A	120	ASN
1	4-A	138	ASN
1	4-A	201	ASN
1	4-A	238	GLN
1	4-A	239	ASN

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Mol	Chain	Res	Type
1	4-A	268	GLN
1	4-A	279	HIS
1	4-A	320	ASN
1	4-A	345	ASN
1	4-A	460	ASN
1	4-A	462	ASN
1	4-B	50	GLN
1	4-B	68	GLN
1	4-B	75	ASN
1	4-B	138	ASN
1	4-B	140	HIS
1	4-B	152	ASN
1	4-B	235	HIS
1	4-B	268	GLN
1	4-B	274	GLN
1	4-B	279	HIS
1	5-A	10	GLN
1	5-A	50	GLN
1	5-A	68	GLN
1	5-A	75	ASN
1	5-A	158	HIS
1	5-A	238	GLN
1	5-A	279	HIS
1	5-A	369	GLN
1	5-A	388	ASN
1	5-B	50	GLN
1	5-B	68	GLN
1	5-B	86	ASN
1	5-B	135	ASN
1	5-B	152	ASN
1	5-B	162	GLN
1	5-B	211	GLN
1	5-B	238	GLN
1	5-B	241	ASN
1	5-B	274	GLN
1	5-B	279	HIS
1	5-B	350	ASN
1	5-B	462	ASN
1	6-A	50	GLN
1	6-A	86	ASN
1	6-A	135	ASN
1	6-A	138	ASN

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Mol	Chain	Res	Type
1	6-A	162	GLN
1	6-A	239	ASN
1	6-A	268	GLN
1	6-A	274	GLN
1	6-A	331	GLN
1	6-A	345	ASN
1	6-A	369	GLN
1	6-A	388	ASN
1	6-A	460	ASN
1	6-A	464	ASN
1	6-B	50	GLN
1	6-B	75	ASN
1	6-B	138	ASN
1	6-B	152	ASN
1	6-B	201	ASN
1	6-B	295	ASN
1	7-A	50	GLN
1	7-A	75	ASN
1	7-A	120	ASN
1	7-A	138	ASN
1	7-A	162	GLN
1	7-A	241	ASN
1	7-A	268	GLN
1	7-A	274	GLN
1	7-A	279	HIS
1	7-A	462	ASN
1	7-B	75	ASN
1	7-B	138	ASN
1	7-B	220	ASN
1	7-B	293	ASN
1	8-A	7	ASN
1	8-A	138	ASN
1	8-A	140	HIS
1	8-A	158	HIS
1	8-A	238	GLN
1	8-A	460	ASN
1	8-B	50	GLN
1	8-B	138	ASN
1	8-B	152	ASN
1	8-B	162	GLN
1	8-B	220	ASN
1	8-B	293	ASN

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Mol	Chain	Res	Type
1	8-B	295	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	460/469 (98%)	2.91	319 (69%) 0 0	1, 3, 6, 8	460 (100%)
1	1-B	455/469 (97%)	2.46	265 (58%) 0 0	1, 2, 5, 7	455 (100%)
1	2-A	0/469	-	-	-	-
1	2-B	0/469	-	-	-	-
1	3-A	0/469	-	-	-	-
1	3-B	0/469	-	-	-	-
1	4-A	0/469	-	-	-	-
1	4-B	0/469	-	-	-	-
1	5-A	0/469	-	-	-	-
1	5-B	0/469	-	-	-	-
1	6-A	0/469	-	-	-	-
1	6-B	0/469	-	-	-	-
1	7-A	0/469	-	-	-	-
1	7-B	0/469	-	-	-	-
1	8-A	0/469	-	-	-	-
1	8-B	0/469	-	-	-	-
All	All	915/7504 (12%)	2.69	584 (63%) 0 0	1, 3, 6, 8	915 (100%)

All (584) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	66	VAL	10.0
1	1-B	96	THR	9.1
1	1-A	8	LEU	9.0
1	1-B	146	ILE	8.4
1	1-A	273	ALA	8.0
1	1-A	265	GLY	7.8
1	1-A	70	VAL	7.7
1	1-B	87	GLY	7.4
1	1-B	8	LEU	7.3
1	1-A	443	ALA	7.3

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Mol	Chain	Res	Type	RSRZ
1	1-B	92	THR	7.2
1	1-A	24	SER	7.0
1	1-A	387	THR	6.9
1	1-B	145	LYS	6.8
1	1-A	252	LEU	6.7
1	1-A	379	PHE	6.7
1	1-A	7	ASN	6.6
1	1-A	378	GLY	6.6
1	1-A	189	PRO	6.6
1	1-B	95	CYS	6.5
1	1-B	467	GLU	6.5
1	1-A	469	LEU	6.4
1	1-A	56	ILE	6.2
1	1-B	44	ILE	6.2
1	1-B	143	THR	6.1
1	1-B	147	VAL	6.1
1	1-B	237	ILE	6.1
1	1-A	44	ILE	6.0
1	1-B	173	PHE	6.0
1	1-A	54	ASP	6.0
1	1-A	59	PRO	5.9
1	1-A	51	THR	5.9
1	1-A	283	PHE	5.8
1	1-A	155	VAL	5.8
1	1-B	448	VAL	5.8
1	1-B	324	VAL	5.7
1	1-A	67	SER	5.7
1	1-B	466	PRO	5.7
1	1-B	298	TRP	5.6
1	1-A	251	THR	5.6
1	1-A	461	LYS	5.6
1	1-B	9	PRO	5.6
1	1-A	46	TRP	5.5
1	1-A	446	SER	5.5
1	1-A	39	GLY	5.5
1	1-A	114	ILE	5.4
1	1-A	324	VAL	5.4
1	1-A	444	ALA	5.3
1	1-A	64	THR	5.3
1	1-B	150	TYR	5.3
1	1-B	438	GLY	5.3
1	1-A	210	SER	5.3

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Mol	Chain	Res	Type	RSRZ
1	1-B	244	CYS	5.3
1	1-B	430	PHE	5.3
1	1-B	375	LEU	5.2
1	1-A	253	ALA	5.2
1	1-B	144	HIS	5.2
1	1-B	174	VAL	5.2
1	1-A	69	ASP	5.1
1	1-B	140	HIS	5.1
1	1-B	152	ASN	5.0
1	1-A	286	ILE	5.0
1	1-A	52	PRO	5.0
1	1-A	30	ILE	5.0
1	1-A	146	ILE	5.0
1	1-A	385	ALA	5.0
1	1-A	61	GLU	5.0
1	1-A	68	GLN	4.9
1	1-B	37	LEU	4.9
1	1-B	428	VAL	4.9
1	1-A	262	SER	4.8
1	1-A	87	GLY	4.8
1	1-A	376	VAL	4.8
1	1-A	347	ILE	4.8
1	1-B	429	TRP	4.8
1	1-B	308	VAL	4.8
1	1-B	407	LEU	4.8
1	1-A	358	PRO	4.7
1	1-A	272	ILE	4.7
1	1-B	91	THR	4.7
1	1-A	351	VAL	4.6
1	1-B	376	VAL	4.6
1	1-B	49	ILE	4.6
1	1-B	11	LEU	4.6
1	1-B	372	LEU	4.6
1	1-A	71	ALA	4.6
1	1-A	111	LEU	4.6
1	1-B	18	LEU	4.6
1	1-A	466	PRO	4.6
1	1-B	180	GLY	4.6
1	1-A	62	LYS	4.5
1	1-B	149	LYS	4.5
1	1-A	231	THR	4.5
1	1-A	112	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	1-A	126	GLY	4.5
1	1-B	90	GLY	4.5
1	1-A	9	PRO	4.5
1	1-A	19	THR	4.5
1	1-B	137	PHE	4.4
1	1-A	60	TYR	4.4
1	1-A	260	LEU	4.4
1	1-B	321	PRO	4.4
1	1-A	123	ASN	4.4
1	1-A	58	VAL	4.4
1	1-A	209	LEU	4.4
1	1-A	267	VAL	4.4
1	1-A	375	LEU	4.4
1	1-A	467	GLU	4.4
1	1-B	454	ASP	4.4
1	1-A	463	ILE	4.4
1	1-A	151	THR	4.4
1	1-A	55	GLU	4.4
1	1-A	121	LEU	4.3
1	1-B	450	LEU	4.3
1	1-A	255	VAL	4.3
1	1-B	463	ILE	4.3
1	1-B	346	ALA	4.3
1	1-A	313	LEU	4.3
1	1-A	57	VAL	4.2
1	1-B	136	SER	4.2
1	1-B	300	ASN	4.2
1	1-A	388	ASN	4.2
1	1-B	10	GLN	4.2
1	1-A	65	PRO	4.2
1	1-A	450	LEU	4.2
1	1-B	468	ASP	4.2
1	1-A	53	THR	4.2
1	1-A	76	LEU	4.2
1	1-A	325	ASP	4.2
1	1-A	390	SER	4.1
1	1-B	100	SER	4.1
1	1-A	82	VAL	4.1
1	1-A	349	VAL	4.1
1	1-B	326	GLY	4.1
1	1-A	125	TYR	4.1
1	1-A	127	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	1-B	464	ASN	4.1
1	1-A	275	VAL	4.1
1	1-A	312	ALA	4.1
1	1-A	263	TYR	4.1
1	1-B	141	ASP	4.1
1	1-A	285	SER	4.1
1	1-B	240	LYS	4.1
1	1-B	305	LYS	4.1
1	1-A	442	VAL	4.0
1	1-A	276	PRO	4.0
1	1-A	266	LYS	4.0
1	1-B	282	GLU	4.0
1	1-A	77	LEU	4.0
1	1-A	104	VAL	4.0
1	1-A	277	ASP	4.0
1	1-A	416	ILE	4.0
1	1-A	420	ASP	4.0
1	1-B	261	ILE	4.0
1	1-B	275	VAL	4.0
1	1-B	408	SER	4.0
1	1-A	191	GLY	4.0
1	1-A	224	LEU	4.0
1	1-A	394	ILE	4.0
1	1-B	217	PHE	4.0
1	1-B	452	ILE	4.0
1	1-A	350	ASN	4.0
1	1-A	354	SER	4.0
1	1-A	462	ASN	4.0
1	1-A	207	THR	3.9
1	1-B	89	LEU	3.9
1	1-A	237	ILE	3.9
1	1-A	445	LYS	3.9
1	1-B	27	SER	3.9
1	1-B	142	ASP	3.9
1	1-B	169	VAL	3.9
1	1-B	167	ARG	3.8
1	1-B	295	ASN	3.8
1	1-A	13	SER	3.8
1	1-A	124	LYS	3.8
1	1-B	458	VAL	3.8
1	1-B	32	LEU	3.8
1	1-B	17	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	1-A	75	ASN	3.8
1	1-A	318	ILE	3.8
1	1-A	452	ILE	3.8
1	1-B	327	VAL	3.8
1	1-A	153	SER	3.8
1	1-B	425	SER	3.8
1	1-A	204	LYS	3.8
1	1-B	184	LYS	3.8
1	1-B	125	TYR	3.8
1	1-B	170	ALA	3.8
1	1-B	310	ALA	3.8
1	1-A	102	ILE	3.8
1	1-A	289	PHE	3.8
1	1-A	455	ARG	3.8
1	1-A	389	PRO	3.7
1	1-A	31	SER	3.7
1	1-A	380	VAL	3.7
1	1-A	10	GLN	3.7
1	1-A	264	GLU	3.7
1	1-B	148	GLU	3.7
1	1-A	226	ALA	3.7
1	1-A	310	ALA	3.7
1	1-A	279	HIS	3.7
1	1-A	228	VAL	3.7
1	1-B	183	ASP	3.7
1	1-A	113	LEU	3.6
1	1-B	278	GLU	3.6
1	1-B	151	THR	3.6
1	1-B	182	THR	3.6
1	1-B	276	PRO	3.6
1	1-A	211	GLN	3.6
1	1-A	281	ASN	3.6
1	1-B	322	LYS	3.6
1	1-B	462	ASN	3.6
1	1-A	11	LEU	3.6
1	1-A	436	LEU	3.6
1	1-A	84	LYS	3.6
1	1-B	179	LYS	3.6
1	1-A	348	GLY	3.6
1	1-A	287	GLU	3.6
1	1-A	35	ARG	3.6
1	1-B	360	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	1-A	460	ASN	3.5
1	1-A	49	ILE	3.5
1	1-B	286	ILE	3.5
1	1-A	411	LYS	3.5
1	1-A	357	LEU	3.5
1	1-B	328	LYS	3.5
1	1-A	137	PHE	3.5
1	1-B	126	GLY	3.5
1	1-A	132	VAL	3.5
1	1-A	230	LEU	3.5
1	1-A	438	GLY	3.5
1	1-B	431	GLY	3.5
1	1-A	6	GLU	3.4
1	1-A	244	CYS	3.4
1	1-B	352	PRO	3.4
1	1-B	35	ARG	3.4
1	1-A	234	LYS	3.4
1	1-A	447	GLY	3.4
1	1-B	203	GLY	3.4
1	1-B	436	LEU	3.4
1	1-A	271	GLU	3.4
1	1-A	326	GLY	3.4
1	1-A	430	PHE	3.4
1	1-B	50	GLN	3.4
1	1-A	200	MET	3.4
1	1-A	150	TYR	3.4
1	1-A	274	GLN	3.4
1	1-A	115	VAL	3.4
1	1-A	448	VAL	3.4
1	1-B	351	VAL	3.4
1	1-A	345	ASN	3.4
1	1-B	406	PHE	3.4
1	1-B	36	TYR	3.3
1	1-A	464	ASN	3.3
1	1-B	133	LEU	3.3
1	1-A	208	PHE	3.3
1	1-B	103	GLU	3.3
1	1-B	112	ASP	3.3
1	1-A	27	SER	3.3
1	1-A	320	ASN	3.3
1	1-B	13	SER	3.3
1	1-A	340	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	403	VAL	3.3
1	1-B	435	VAL	3.3
1	1-B	457	VAL	3.3
1	1-A	108	LEU	3.3
1	1-A	233	LEU	3.3
1	1-A	372	LEU	3.3
1	1-A	173	PHE	3.3
1	1-B	135	ASN	3.3
1	1-B	114	ILE	3.3
1	1-A	15	VAL	3.3
1	1-A	152	ASN	3.3
1	1-B	299	VAL	3.2
1	1-A	367	LEU	3.2
1	1-B	356	PHE	3.2
1	1-B	30	ILE	3.2
1	1-A	201	ASN	3.2
1	1-A	362	SER	3.2
1	1-B	21	MET	3.2
1	1-A	268	GLN	3.2
1	1-A	440	VAL	3.2
1	1-A	457	VAL	3.2
1	1-A	37	LEU	3.2
1	1-B	200	MET	3.2
1	1-B	313	LEU	3.2
1	1-B	377	ASP	3.2
1	1-A	187	TRP	3.1
1	1-A	384	LYS	3.1
1	1-A	434	ILE	3.1
1	1-A	456	ALA	3.1
1	1-B	33	VAL	3.1
1	1-B	29	PHE	3.1
1	1-B	277	ASP	3.1
1	1-B	12	LYS	3.1
1	1-A	63	MET	3.1
1	1-A	28	GLY	3.1
1	1-A	147	VAL	3.1
1	1-A	199	LEU	3.1
1	1-A	468	ASP	3.1
1	1-A	74	LYS	3.1
1	1-B	99	LYS	3.1
1	1-A	374	THR	3.1
1	1-A	381	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	1-A	428	VAL	3.1
1	1-B	368	VAL	3.1
1	1-A	292	PHE	3.1
1	1-A	73	THR	3.1
1	1-A	278	GLU	3.1
1	1-B	242	GLU	3.1
1	1-A	94	GLY	3.1
1	1-A	97	GLY	3.1
1	1-B	186	GLY	3.1
1	1-A	118	ILE	3.0
1	1-B	304	ILE	3.0
1	1-B	373	TYR	3.0
1	1-B	281	ASN	3.0
1	1-A	465	GLY	3.0
1	1-B	330	LEU	3.0
1	1-B	366	LEU	3.0
1	1-A	101	VAL	3.0
1	1-B	309	GLU	3.0
1	1-A	352	PRO	3.0
1	1-A	256	LYS	3.0
1	1-A	361	ALA	3.0
1	1-A	327	VAL	3.0
1	1-B	255	VAL	3.0
1	1-A	47	SER	3.0
1	1-B	423	LYS	3.0
1	1-A	205	LEU	2.9
1	1-A	330	LEU	2.9
1	1-A	247	VAL	2.9
1	1-A	415	SER	2.9
1	1-A	145	LYS	2.9
1	1-A	284	LYS	2.9
1	1-A	437	LYS	2.9
1	1-A	167	ARG	2.9
1	1-B	405	THR	2.9
1	1-B	196	PHE	2.9
1	1-B	343	PHE	2.9
1	1-B	400	PHE	2.9
1	1-A	413	ILE	2.9
1	1-A	131	LEU	2.9
1	1-B	181	LYS	2.9
1	1-B	66	VAL	2.9
1	1-B	379	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	1-A	83	LEU	2.9
1	1-A	236	LEU	2.9
1	1-A	419	LEU	2.9
1	1-B	447	GLY	2.9
1	1-A	190	PRO	2.9
1	1-B	453	PRO	2.9
1	1-A	106	ASP	2.9
1	1-A	171	ASP	2.9
1	1-B	23	GLU	2.9
1	1-A	301	LEU	2.9
1	1-A	161	ASN	2.8
1	1-A	435	VAL	2.8
1	1-B	15	VAL	2.8
1	1-B	381	THR	2.8
1	1-B	303	ALA	2.8
1	1-B	323	GLU	2.8
1	1-B	46	TRP	2.8
1	1-B	56	ILE	2.8
1	1-B	121	LEU	2.8
1	1-B	97	GLY	2.8
1	1-B	19	THR	2.8
1	1-A	319	PRO	2.8
1	1-B	424	VAL	2.8
1	1-B	446	SER	2.8
1	1-A	239	ASN	2.8
1	1-B	426	GLY	2.8
1	1-B	113	LEU	2.8
1	1-A	290	LYS	2.8
1	1-B	109	THR	2.8
1	1-A	72	GLU	2.8
1	1-B	442	VAL	2.8
1	1-B	412	SER	2.8
1	1-A	360	LYS	2.8
1	1-B	434	ILE	2.8
1	1-A	414	PRO	2.8
1	1-A	453	PRO	2.8
1	1-A	218	VAL	2.8
1	1-A	373	TYR	2.7
1	1-A	382	ARG	2.7
1	1-B	456	ALA	2.7
1	1-A	439	LYS	2.7
1	1-B	80	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	1-B	236	LEU	2.7
1	1-A	232	ILE	2.7
1	1-B	325	ASP	2.7
1	1-A	421	SER	2.7
1	1-B	178	SER	2.7
1	1-A	158	HIS	2.7
1	1-A	78	ASP	2.7
1	1-A	269	LEU	2.7
1	1-A	321	PRO	2.7
1	1-A	227	ILE	2.7
1	1-B	459	GLU	2.7
1	1-A	404	ALA	2.7
1	1-B	53	THR	2.7
1	1-A	50	GLN	2.7
1	1-B	24	SER	2.7
1	1-A	240	LYS	2.7
1	1-B	78	ASP	2.6
1	1-B	165	TYR	2.6
1	1-A	386	ARG	2.6
1	1-B	410	PHE	2.6
1	1-B	451	GLU	2.6
1	1-A	393	SER	2.6
1	1-B	230	LEU	2.6
1	1-A	129	VAL	2.6
1	1-A	280	VAL	2.6
1	1-B	193	GLY	2.6
1	1-B	280	VAL	2.6
1	1-A	311	ASP	2.6
1	1-B	427	ASP	2.6
1	1-B	117	GLN	2.6
1	1-A	45	GLU	2.6
1	1-A	185	GLU	2.6
1	1-A	116	ILE	2.6
1	1-A	254	ASP	2.6
1	1-B	171	ASP	2.6
1	1-A	451	GLU	2.6
1	1-A	458	VAL	2.6
1	1-A	423	LYS	2.6
1	1-B	74	LYS	2.6
1	1-B	124	LYS	2.6
1	1-B	190	PRO	2.6
1	1-A	366	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	1-B	108	LEU	2.6
1	1-A	20	GLU	2.6
1	1-B	256	LYS	2.6
1	1-B	329	VAL	2.6
1	1-A	441	THR	2.6
1	1-B	159	THR	2.6
1	1-B	106	ASP	2.5
1	1-A	90	GLY	2.5
1	1-B	88	GLY	2.5
1	1-B	128	LYS	2.5
1	1-B	317	ILE	2.5
1	1-A	138	ASN	2.5
1	1-A	170	ALA	2.5
1	1-A	339	ALA	2.5
1	1-B	443	ALA	2.5
1	1-A	432	SER	2.5
1	1-A	195	VAL	2.5
1	1-A	188	TYR	2.5
1	1-A	396	LEU	2.5
1	1-B	76	LEU	2.5
1	1-B	107	GLY	2.5
1	1-A	238	GLN	2.5
1	1-B	251	THR	2.5
1	1-B	369	GLN	2.5
1	1-B	374	THR	2.5
1	1-A	371	ASP	2.5
1	1-A	377	ASP	2.5
1	1-A	36	TYR	2.5
1	1-A	193	GLY	2.5
1	1-B	455	ARG	2.5
1	1-A	261	ILE	2.5
1	1-A	119	GLU	2.5
1	1-B	176	TRP	2.5
1	1-B	404	ALA	2.5
1	1-A	368	VAL	2.5
1	1-B	16	ASP	2.5
1	1-A	422	LEU	2.4
1	1-B	270	LEU	2.4
1	1-A	323	GLU	2.4
1	1-B	34	SER	2.4
1	1-B	432	SER	2.4
1	1-B	318	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	1-A	14	ALA	2.4
1	1-A	314	LYS	2.4
1	1-B	349	VAL	2.4
1	1-B	417	VAL	2.4
1	1-B	161	ASN	2.4
1	1-B	239	ASN	2.4
1	1-A	38	SER	2.4
1	1-A	270	LEU	2.4
1	1-B	31	SER	2.4
1	1-B	297	LEU	2.4
1	1-A	410	PHE	2.4
1	1-B	164	LYS	2.4
1	1-B	14	ALA	2.4
1	1-A	355	ARG	2.4
1	1-A	398	PRO	2.4
1	1-A	298	TRP	2.4
1	1-B	359	VAL	2.4
1	1-A	426	GLY	2.4
1	1-A	110	PHE	2.4
1	1-A	291	ILE	2.4
1	1-B	265	GLY	2.4
1	1-B	403	VAL	2.4
1	1-A	26	LYS	2.4
1	1-A	288	LYS	2.4
1	1-B	131	LEU	2.3
1	1-B	205	LEU	2.3
1	1-B	409	ARG	2.3
1	1-B	51	THR	2.3
1	1-B	54	ASP	2.3
1	1-B	311	ASP	2.3
1	1-A	429	TRP	2.3
1	1-A	23	GLU	2.3
1	1-A	395	GLU	2.3
1	1-B	77	LEU	2.3
1	1-A	259	THR	2.3
1	1-B	157	ILE	2.3
1	1-A	221	SER	2.3
1	1-B	202	SER	2.3
1	1-A	359	VAL	2.3
1	1-A	341	ARG	2.3
1	1-B	70	VAL	2.3
1	1-A	154	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	1-B	301	LEU	2.3
1	1-B	332	LEU	2.3
1	1-B	387	THR	2.3
1	1-B	60	TYR	2.2
1	1-B	243	TYR	2.2
1	1-A	433	SER	2.2
1	1-B	285	SER	2.2
1	1-B	232	ILE	2.2
1	1-B	238	GLN	2.2
1	1-B	195	VAL	2.2
1	1-B	216	VAL	2.2
1	1-B	111	LEU	2.2
1	1-A	86	ASN	2.2
1	1-A	250	LYS	2.2
1	1-A	143	THR	2.2
1	1-B	22	SER	2.2
1	1-B	98	PRO	2.2
1	1-B	416	ILE	2.2
1	1-B	341	ARG	2.2
1	1-B	287	GLU	2.2
1	1-A	424	VAL	2.2
1	1-A	202	SER	2.2
1	1-A	144	HIS	2.1
1	1-A	196	PHE	2.1
1	1-A	295	ASN	2.1
1	1-A	342	PHE	2.1
1	1-B	86	ASN	2.1
1	1-B	345	ASN	2.1
1	1-B	172	GLU	2.1
1	1-A	96	THR	2.1
1	1-B	168	VAL	2.1
1	1-B	127	CYS	2.1
1	1-A	328	LYS	2.1
1	1-B	26	LYS	2.1
1	1-B	214	GLU	2.1
1	1-B	221	SER	2.1
1	1-B	101	VAL	2.1
1	1-A	128	LYS	2.1
1	1-B	319	PRO	2.1
1	1-A	338	ALA	2.1
1	1-B	444	ALA	2.1
1	1-A	142	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	1-A	454	ASP	2.1
1	1-B	461	LYS	2.1
1	1-B	175	PRO	2.1
1	1-A	85	LEU	2.1
1	1-A	95	CYS	2.1
1	1-B	45	GLU	2.0
1	1-A	22	SER	2.0
1	1-B	266	LYS	2.0
1	1-B	354	SER	2.0
1	1-B	93	MET	2.0
1	1-A	225	GLY	2.0
1	1-B	120	ASN	2.0
1	1-B	177	PRO	2.0
1	1-B	187	TRP	2.0
1	1-B	396	LEU	2.0
1	1-A	194	ASP	2.0
1	1-A	229	ASP	2.0
1	1-A	25	GLU	2.0
1	1-A	425	SER	2.0
1	1-B	153	SER	2.0
1	1-A	157	ILE	2.0
1	1-B	279	HIS	2.0
1	1-A	107	GLY	2.0
1	1-A	431	GLY	2.0
1	1-B	122	ASN	2.0
1	1-B	465	GLY	2.0
1	1-B	129	VAL	2.0
1	1-B	380	VAL	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 oligosaccharides 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.