



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 11:30 PM EDT

PDB ID : 4C5U  
Title : Structural Investigations into the Stereochemistry and Activity of a Phenylalanine-2,3-Aminomutase from *Taxus chinensis*  
Authors : Wybenga, G.G.; Szymanski, W.; Wu, B.; Feringa, B.L.; Janssen, D.B.; Dijkstra, B.W.  
Deposited on : 2013-09-16  
Resolution : 2.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

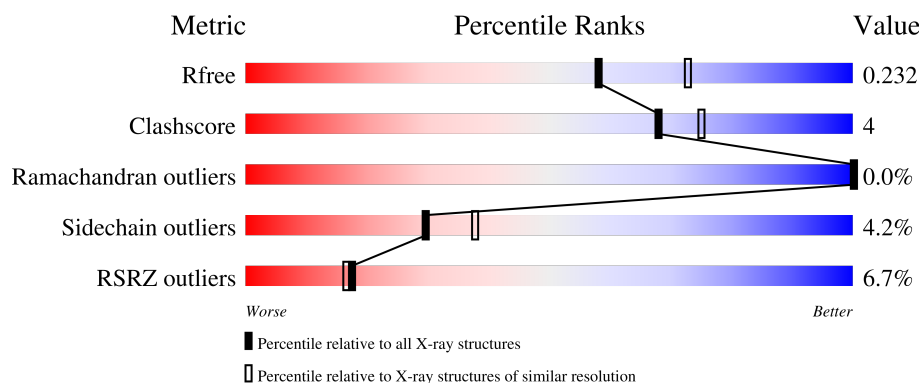
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


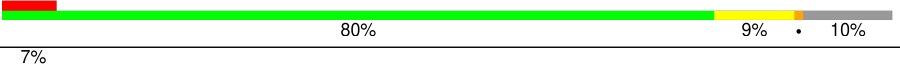
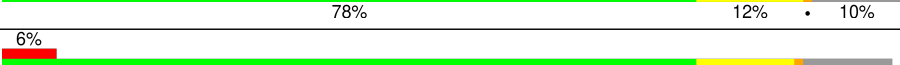

The reported resolution of this entry is 2.19 Å.

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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	A	707	
1	B	707	
1	C	707	
1	D	707	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19779 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 PHENYLALANINE AMMONIA-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	641	Total	C	N	O	S	0	0	0
			4962	3147	855	937	23			
1	B	636	Total	C	N	O	S	0	0	0
			4922	3120	847	932	23			
1	C	639	Total	C	N	O	S	0	0	0
			4941	3133	853	932	23			
1	D	636	Total	C	N	O	S	0	0	0
			4917	3121	848	925	23			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q68G84
A	-18	GLY	-	expression tag	UNP Q68G84
A	-17	SER	-	expression tag	UNP Q68G84
A	-16	SER	-	expression tag	UNP Q68G84
A	-15	HIS	-	expression tag	UNP Q68G84
A	-14	HIS	-	expression tag	UNP Q68G84
A	-13	HIS	-	expression tag	UNP Q68G84
A	-12	HIS	-	expression tag	UNP Q68G84
A	-11	HIS	-	expression tag	UNP Q68G84
A	-10	HIS	-	expression tag	UNP Q68G84
A	-9	SER	-	expression tag	UNP Q68G84
A	-8	SER	-	expression tag	UNP Q68G84
A	-7	GLY	-	expression tag	UNP Q68G84
A	-6	LEU	-	expression tag	UNP Q68G84
A	-5	VAL	-	expression tag	UNP Q68G84
A	-4	PRO	-	expression tag	UNP Q68G84
A	-3	ARG	-	expression tag	UNP Q68G84
A	-2	GLY	-	expression tag	UNP Q68G84
A	-1	SER	-	expression tag	UNP Q68G84
A	0	HIS	-	expression tag	UNP Q68G84
A	322	ALA	TYR	engineered mutation	UNP Q68G84

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP Q68G84
B	-18	GLY	-	expression tag	UNP Q68G84
B	-17	SER	-	expression tag	UNP Q68G84
B	-16	SER	-	expression tag	UNP Q68G84
B	-15	HIS	-	expression tag	UNP Q68G84
B	-14	HIS	-	expression tag	UNP Q68G84
B	-13	HIS	-	expression tag	UNP Q68G84
B	-12	HIS	-	expression tag	UNP Q68G84
B	-11	HIS	-	expression tag	UNP Q68G84
B	-10	HIS	-	expression tag	UNP Q68G84
B	-9	SER	-	expression tag	UNP Q68G84
B	-8	SER	-	expression tag	UNP Q68G84
B	-7	GLY	-	expression tag	UNP Q68G84
B	-6	LEU	-	expression tag	UNP Q68G84
B	-5	VAL	-	expression tag	UNP Q68G84
B	-4	PRO	-	expression tag	UNP Q68G84
B	-3	ARG	-	expression tag	UNP Q68G84
B	-2	GLY	-	expression tag	UNP Q68G84
B	-1	SER	-	expression tag	UNP Q68G84
B	0	HIS	-	expression tag	UNP Q68G84
B	322	ALA	TYR	engineered mutation	UNP Q68G84
C	-19	MET	-	expression tag	UNP Q68G84
C	-18	GLY	-	expression tag	UNP Q68G84
C	-17	SER	-	expression tag	UNP Q68G84
C	-16	SER	-	expression tag	UNP Q68G84
C	-15	HIS	-	expression tag	UNP Q68G84
C	-14	HIS	-	expression tag	UNP Q68G84
C	-13	HIS	-	expression tag	UNP Q68G84
C	-12	HIS	-	expression tag	UNP Q68G84
C	-11	HIS	-	expression tag	UNP Q68G84
C	-10	HIS	-	expression tag	UNP Q68G84
C	-9	SER	-	expression tag	UNP Q68G84
C	-8	SER	-	expression tag	UNP Q68G84
C	-7	GLY	-	expression tag	UNP Q68G84
C	-6	LEU	-	expression tag	UNP Q68G84
C	-5	VAL	-	expression tag	UNP Q68G84
C	-4	PRO	-	expression tag	UNP Q68G84
C	-3	ARG	-	expression tag	UNP Q68G84
C	-2	GLY	-	expression tag	UNP Q68G84
C	-1	SER	-	expression tag	UNP Q68G84
C	0	HIS	-	expression tag	UNP Q68G84
C	322	ALA	TYR	engineered mutation	UNP Q68G84

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	-19	MET	-	expression tag	UNP Q68G84
D	-18	GLY	-	expression tag	UNP Q68G84
D	-17	SER	-	expression tag	UNP Q68G84
D	-16	SER	-	expression tag	UNP Q68G84
D	-15	HIS	-	expression tag	UNP Q68G84
D	-14	HIS	-	expression tag	UNP Q68G84
D	-13	HIS	-	expression tag	UNP Q68G84
D	-12	HIS	-	expression tag	UNP Q68G84
D	-11	HIS	-	expression tag	UNP Q68G84
D	-10	HIS	-	expression tag	UNP Q68G84
D	-9	SER	-	expression tag	UNP Q68G84
D	-8	SER	-	expression tag	UNP Q68G84
D	-7	GLY	-	expression tag	UNP Q68G84
D	-6	LEU	-	expression tag	UNP Q68G84
D	-5	VAL	-	expression tag	UNP Q68G84
D	-4	PRO	-	expression tag	UNP Q68G84
D	-3	ARG	-	expression tag	UNP Q68G84
D	-2	GLY	-	expression tag	UNP Q68G84
D	-1	SER	-	expression tag	UNP Q68G84
D	0	HIS	-	expression tag	UNP Q68G84
D	322	ALA	TYR	engineered mutation	UNP Q68G84

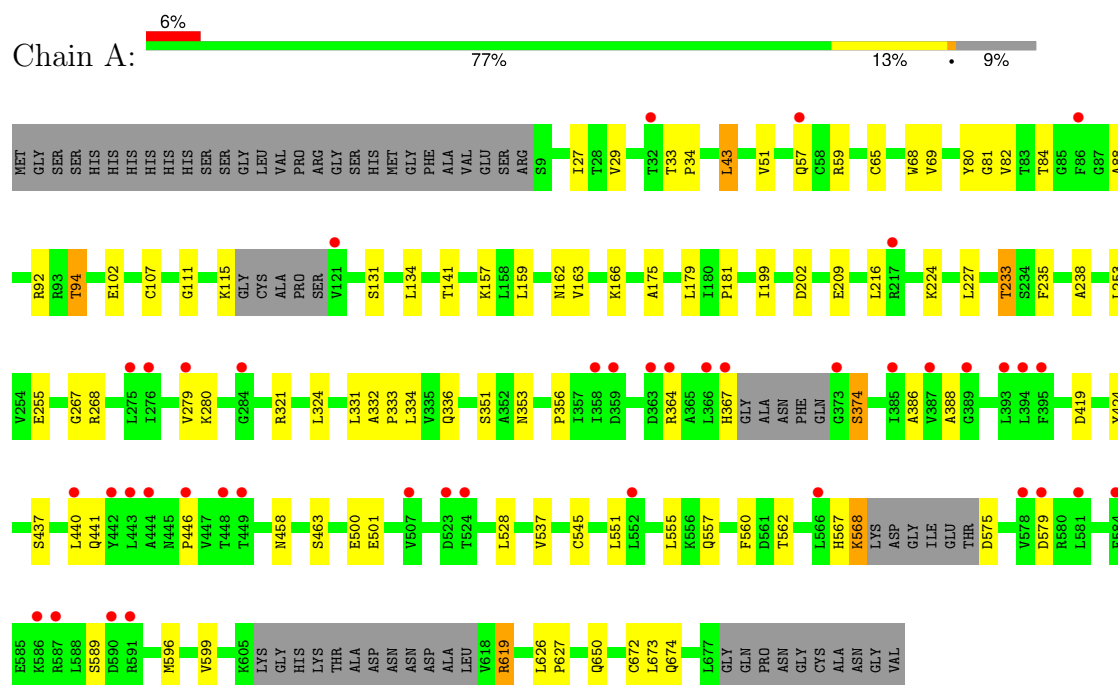
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	O	0	0
			15	15		
2	B	6	Total	O	0	0
			6	6		
2	C	10	Total	O	0	0
			10	10		
2	D	6	Total	O	0	0
			6	6		

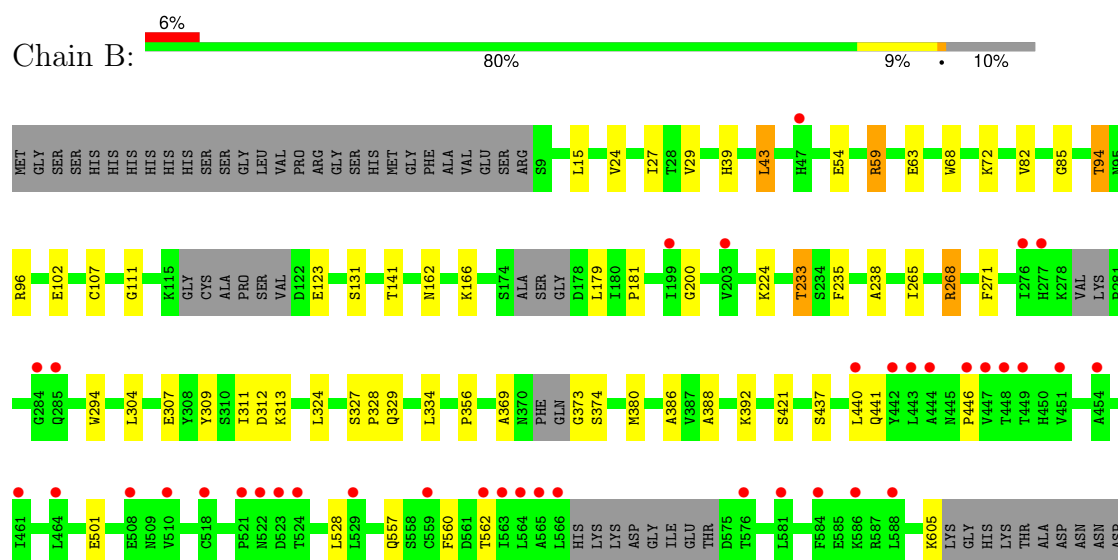
### 3 Residue-property plots

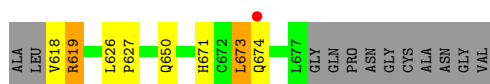
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PHENYLALANINE AMMONIA-LYASE

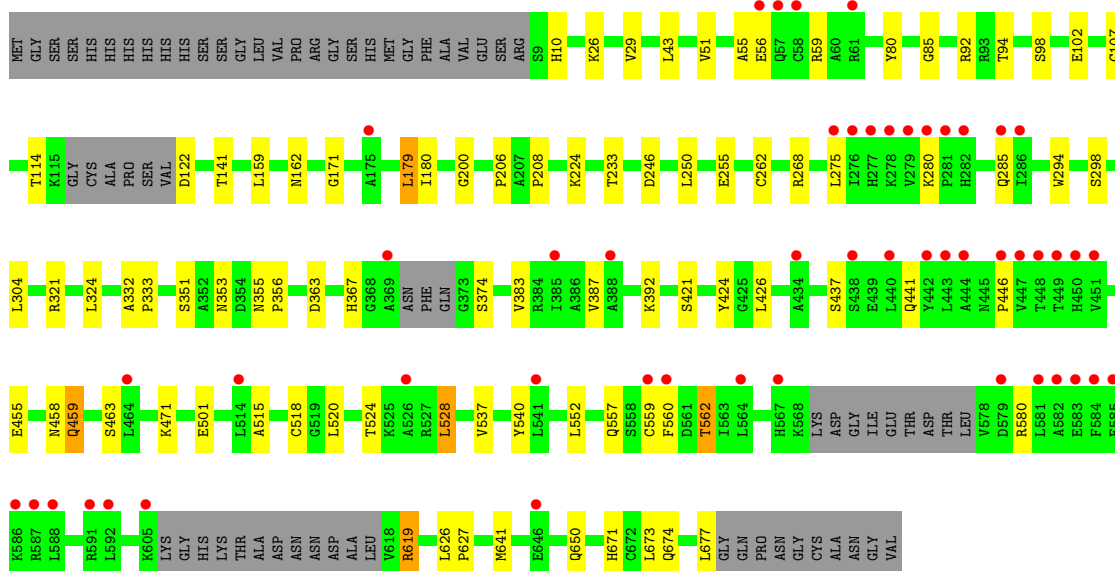
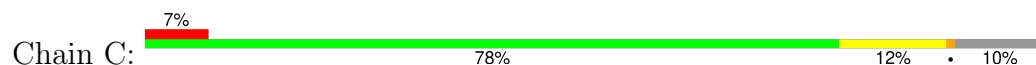


#### • Molecule 1: PHENYLALANINE AMMONIA-LYASE

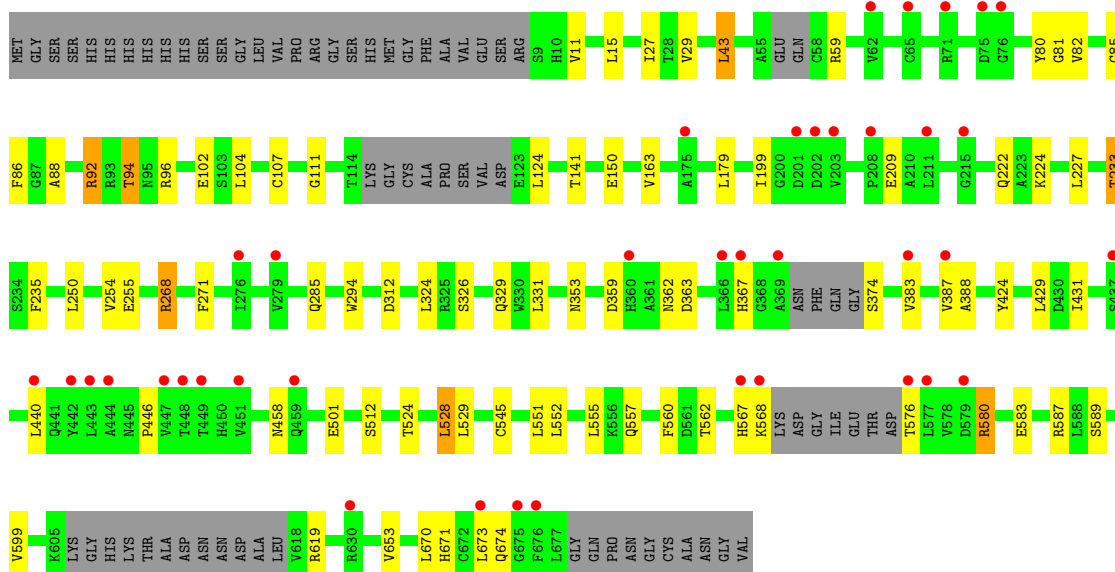
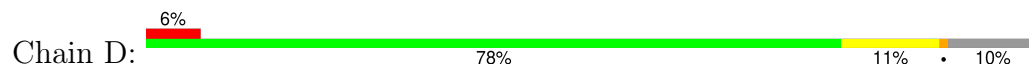




● Molecule 1: PHENYLALANINE AMMONIA-LYASE



● Molecule 1: PHENYLALANINE AMMONIA-LYASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.48Å 147.27Å 99.77Å 90.00° 99.80° 90.00°	Depositor
Resolution (Å)	48.38 – 2.19 48.38 – 2.19	Depositor EDS
% Data completeness (in resolution range)	94.3 (48.38-2.19) 98.1 (48.38-2.19)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.83 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.189 , 0.224 0.194 , 0.232	Depositor DCC
$R_{free}$ test set	7178 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 34.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
Reported twinning fraction	0.865 for H, K, L 0.135 for L, -K, H	Depositor
Outliers	1 of 141777 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19779	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.57	1/5045 (0.0%)	0.69	1/6843 (0.0%)
1	B	0.54	2/5002 (0.0%)	0.65	1/6782 (0.0%)
1	C	0.55	1/5024 (0.0%)	0.67	1/6813 (0.0%)
1	D	0.55	1/4999 (0.0%)	0.68	0/6780
All	All	0.56	5/20070 (0.0%)	0.67	3/27218 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	294	TRP	CD2-CE2	5.71	1.48	1.41
1	B	68	TRP	CD2-CE2	5.47	1.48	1.41
1	B	294	TRP	CD2-CE2	5.26	1.47	1.41
1	A	68	TRP	CD2-CE2	5.07	1.47	1.41
1	D	294	TRP	CD2-CE2	5.06	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	619	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	619	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	321	ARG	NE-CZ-NH2	-5.37	117.62	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4962	0	5044	50	0
1	B	4922	0	4993	40	0
1	C	4941	0	5021	45	0
1	D	4917	0	5004	40	0
2	A	15	0	0	0	0
2	B	6	0	0	0	0
2	C	10	0	0	0	0
2	D	6	0	0	0	0
All	All	19779	0	20062	151	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 4.

All (151) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:HG12	1:A:141:THR:HG21	1.58	0.85
1:D:580:ARG:HH11	1:D:580:ARG:CG	2.01	0.74
1:A:80:TYR:HB3	1:A:367:HIS:HD2	1.52	0.73
1:B:671:HIS:O	1:B:674:GLN:HG2	1.89	0.72
1:D:29:VAL:HG12	1:D:141:THR:HG21	1.71	0.71
1:B:446:PRO:HD3	1:D:446:PRO:HD3	1.72	0.71
1:A:557:GLN:NE2	1:D:557:GLN:OE1	2.21	0.71
1:C:501:GLU:OE1	1:C:619:ARG:HD2	1.91	0.70
1:B:557:GLN:NE2	1:C:557:GLN:OE1	2.23	0.69
1:A:650:GLN:HG3	1:B:111:GLY:O	1.93	0.68
1:A:80:TYR:HB3	1:A:367:HIS:CD2	2.30	0.66
1:C:224:LYS:HE2	1:C:356:PRO:HD2	1.78	0.65
1:A:43:LEU:HD22	1:A:134:LEU:HD22	1.79	0.64
1:B:224:LYS:HE2	1:B:356:PRO:HD2	1.80	0.63
1:C:515:ALA:HA	1:C:520:LEU:HD12	1.82	0.61
1:D:163:VAL:HG22	1:D:199:ILE:HG12	1.83	0.61
1:B:29:VAL:HG12	1:B:141:THR:HG21	1.82	0.60
1:C:304:LEU:HD11	1:C:619:ARG:HD3	1.84	0.60
1:B:233:THR:HG21	1:B:373:GLY:N	2.15	0.60
1:C:437:SER:O	1:C:441:GLN:HG2	2.02	0.59
1:B:123:GLU:OE1	1:B:166:LYS:HE3	2.05	0.57
1:D:580:ARG:HH11	1:D:580:ARG:HG3	1.68	0.57
1:C:524:THR:HG22	1:C:528:LEU:HD22	1.87	0.56
1:C:29:VAL:HG12	1:C:141:THR:HG21	1.86	0.56
1:C:455:GLU:HB3	1:C:459:GLN:HG3	1.88	0.55
1:A:157:LYS:HD2	1:A:216:LEU:HD21	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:GLY:O	1:C:180:ILE:HD12	2.06	0.55
1:A:374:SER:HA	1:A:463:SER:HB3	1.89	0.54
1:D:82:VAL:HG22	1:D:224:LYS:HB2	1.87	0.54
1:A:501:GLU:OE1	1:A:619:ARG:HD2	2.06	0.54
1:A:446:PRO:HD3	1:C:446:PRO:HD3	1.90	0.54
1:D:671:HIS:O	1:D:674:GLN:HG2	2.08	0.54
1:D:501:GLU:OE1	1:D:619:ARG:HD2	2.08	0.53
1:A:255:GLU:HG2	1:A:331:LEU:HD13	1.91	0.52
1:A:351:SER:HB2	1:C:280:LYS:HA	1.91	0.52
1:A:88:ALA:HB2	1:A:458:ASN:HB2	1.90	0.52
1:A:424:TYR:OH	1:B:85:GLY:HA2	2.10	0.52
1:A:81:GLY:HA3	1:A:227:LEU:HD22	1.92	0.52
1:A:551:LEU:O	1:A:555:LEU:HG	2.10	0.52
1:D:233:THR:HG23	1:D:233:THR:O	2.10	0.51
1:A:321:ARG:HG2	1:C:458:ASN:HA	1.93	0.50
1:C:179:LEU:HD23	1:D:431:ILE:HD13	1.94	0.50
1:A:29:VAL:CG1	1:A:141:THR:HG21	2.36	0.50
1:B:334:LEU:HD22	1:B:386:ALA:HA	1.93	0.50
1:B:327:SER:OG	1:B:328:PRO:HD3	2.12	0.50
1:D:94:THR:HB	1:D:96:ARG:H	1.77	0.50
1:B:265:ILE:HG21	1:B:324:LEU:HD12	1.94	0.49
1:B:388:ALA:HA	1:B:440:LEU:HG	1.94	0.49
1:C:80:TYR:HB3	1:C:367:HIS:CD2	2.48	0.49
1:C:114:THR:OG1	1:C:122:ASP:HB2	2.12	0.49
1:B:15:LEU:HD21	1:B:673:LEU:HD23	1.95	0.49
1:C:285:GLN:HB2	1:C:332:ALA:HB2	1.95	0.49
1:A:332:ALA:HB3	1:A:333:PRO:CD	2.42	0.49
1:C:374:SER:HA	1:C:463:SER:HB2	1.95	0.49
1:B:437:SER:O	1:B:441:GLN:HG2	2.13	0.48
1:D:88:ALA:HB2	1:D:458:ASN:HB2	1.94	0.48
1:C:10:HIS:NE2	1:C:255:GLU:OE1	2.47	0.48
1:A:545:CYS:SG	1:A:589:SER:HA	2.54	0.48
1:A:334:LEU:HD22	1:A:386:ALA:HA	1.95	0.48
1:C:671:HIS:O	1:C:674:GLN:HG2	2.14	0.48
1:C:332:ALA:HB3	1:C:333:PRO:HD3	1.94	0.48
1:B:27:ILE:CD1	1:B:43:LEU:HB2	2.43	0.48
1:B:329:GLN:O	1:D:374:SER:OG	2.27	0.48
1:A:437:SER:O	1:A:441:GLN:HG2	2.13	0.47
1:D:27:ILE:CD1	1:D:43:LEU:HB2	2.44	0.47
1:A:267:GLY:HA3	1:A:324:LEU:HD11	1.96	0.47
1:A:560:PHE:HB2	1:D:560:PHE:HB2	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:TYR:OH	1:D:85:GLY:HA2	2.14	0.47
1:A:579:ASP:OD1	1:D:567:HIS:NE2	2.42	0.47
1:B:501:GLU:OE1	1:B:619:ARG:HD2	2.14	0.47
1:D:429:LEU:HD21	1:D:653:VAL:HG21	1.96	0.47
1:B:131:SER:HB2	1:B:238:ALA:HB1	1.97	0.47
1:A:388:ALA:HA	1:A:440:LEU:HG	1.97	0.47
1:C:383:VAL:O	1:C:387:VAL:HG23	2.14	0.46
1:A:567:HIS:O	1:A:568:LYS:HD3	2.15	0.46
1:B:24:VAL:HG21	1:B:39:HIS:HD2	1.80	0.46
1:A:94:THR:HG23	1:B:421:SER:OG	2.16	0.46
1:D:81:GLY:HA3	1:D:227:LEU:HD22	1.98	0.46
1:B:59:ARG:HD2	1:B:63:GLU:OE1	2.16	0.46
1:A:419:ASP:OD2	1:B:96:ARG:NH1	2.47	0.46
1:D:86:PHE:CD2	1:D:104:LEU:HD13	2.51	0.46
1:A:596:MET:O	1:A:599:VAL:HG12	2.16	0.46
1:C:304:LEU:CD1	1:C:619:ARG:HD3	2.45	0.46
1:A:27:ILE:CD1	1:A:43:LEU:HB2	2.47	0.45
1:A:181:PRO:HB2	1:A:235:PHE:CD2	2.51	0.45
1:C:518:CYS:O	1:C:580:ARG:HD3	2.16	0.45
1:D:268:ARG:O	1:D:271:PHE:HD1	1.99	0.45
1:B:181:PRO:HB2	1:B:235:PHE:CD2	2.51	0.45
1:B:369:ALA:CB	1:D:326:SER:HB3	2.46	0.45
1:A:500:GLU:HG3	1:A:537:VAL:HG12	1.97	0.45
1:C:246:ASP:O	1:C:250:LEU:HG	2.16	0.45
1:C:559:CYS:O	1:C:562:THR:HG22	2.16	0.45
1:D:359:ASP:OD2	1:D:362:ASN:HB2	2.17	0.45
1:A:80:TYR:CB	1:A:367:HIS:CD2	3.00	0.45
1:D:285:GLN:CD	1:D:329:GLN:HG3	2.38	0.45
1:A:163:VAL:HG22	1:A:199:ILE:HG23	1.99	0.44
1:A:224:LYS:O	1:A:224:LYS:HG2	2.18	0.44
1:A:374:SER:HA	1:A:463:SER:CB	2.47	0.44
1:B:560:PHE:CE1	1:C:559:CYS:HB3	2.52	0.44
1:D:383:VAL:O	1:D:387:VAL:HG23	2.17	0.44
1:C:332:ALA:HB3	1:C:333:PRO:CD	2.47	0.44
1:C:51:VAL:HG21	1:C:159:LEU:HD13	2.00	0.44
1:D:11:VAL:O	1:D:15:LEU:HG	2.18	0.44
1:B:560:PHE:HB2	1:C:560:PHE:HB2	2.00	0.44
1:C:421:SER:HB3	1:D:92:ARG:NH1	2.33	0.43
1:C:537:VAL:HA	1:C:540:TYR:CE2	2.53	0.43
1:B:27:ILE:HD12	1:B:43:LEU:HB2	2.01	0.43
1:A:111:GLY:O	1:B:650:GLN:HG3	2.17	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ARG:O	1:B:271:PHE:HD1	2.01	0.43
1:C:206:PRO:HB2	1:C:208:PRO:HD2	1.99	0.43
1:B:309:TYR:O	1:B:313:LYS:HG3	2.19	0.43
1:D:524:THR:HG22	1:D:528:LEU:HD22	2.01	0.43
1:C:426:LEU:HD11	1:C:641:MET:SD	2.58	0.43
1:A:131:SER:CB	1:A:238:ALA:HB1	2.49	0.43
1:D:388:ALA:HA	1:D:440:LEU:HG	2.01	0.43
1:D:512:SER:HB2	1:D:529:LEU:HD21	2.00	0.43
1:A:82:VAL:HG22	1:A:224:LYS:HB2	2.01	0.43
1:D:545:CYS:SG	1:D:589:SER:HA	2.58	0.43
1:A:80:TYR:CB	1:A:367:HIS:HD2	2.27	0.42
1:B:626:LEU:HB3	1:B:627:PRO:HD3	2.01	0.42
1:C:355:ASN:OD1	1:C:356:PRO:HA	2.19	0.42
1:C:55:ALA:O	1:C:59:ARG:HB3	2.20	0.42
1:A:233:THR:HG23	1:A:233:THR:O	2.20	0.42
1:B:307:GLU:O	1:B:311:ILE:HG12	2.19	0.42
1:A:279:VAL:O	1:C:351:SER:HB2	2.18	0.42
1:B:54:GLU:HA	1:B:54:GLU:OE1	2.20	0.41
1:A:332:ALA:O	1:A:336:GLN:HG3	2.20	0.41
1:B:82:VAL:HG22	1:B:224:LYS:HB2	2.01	0.41
1:D:255:GLU:HG2	1:D:331:LEU:HD13	2.03	0.41
1:C:85:GLY:HA2	1:D:424:TYR:OH	2.20	0.41
1:C:262:CYS:HB2	1:C:324:LEU:HD21	2.02	0.41
1:D:124:LEU:HD13	1:D:235:PHE:CE1	2.54	0.41
1:A:626:LEU:HB3	1:A:627:PRO:HD3	2.01	0.41
1:D:250:LEU:O	1:D:254:VAL:HG23	2.21	0.41
1:D:583:GLU:O	1:D:587:ARG:HG3	2.20	0.41
1:A:51:VAL:HG21	1:A:159:LEU:HD13	2.02	0.41
1:A:280:LYS:HA	1:C:351:SER:HB2	2.03	0.41
1:C:626:LEU:N	1:C:627:PRO:HD2	2.36	0.41
1:B:72:LYS:HA	1:B:72:LYS:HD3	1.91	0.41
1:A:33:THR:HA	1:A:34:PRO:HD3	1.87	0.41
1:B:94:THR:HG22	1:B:96:ARG:H	1.85	0.41
1:B:162:ASN:ND2	1:B:200:GLY:HA2	2.36	0.41
1:C:471:LYS:HA	1:C:471:LYS:HD3	1.90	0.41
1:D:80:TYR:HB3	1:D:367:HIS:CD2	2.56	0.41
1:D:551:LEU:O	1:D:555:LEU:HG	2.21	0.40
1:C:650:GLN:HG3	1:D:111:GLY:O	2.22	0.40
1:A:65:CYS:O	1:A:69:VAL:HG23	2.20	0.40
1:B:304:LEU:HD11	1:B:619:ARG:HD3	2.04	0.40
1:C:162:ASN:ND2	1:C:200:GLY:HA2	2.37	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LYS:HE2	1:A:356:PRO:HD2	2.04	0.40
1:B:380:MET:HA	1:B:380:MET:CE	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	631/707 (89%)	616 (98%)	14 (2%)	1 (0%)	47	55
1	B	622/707 (88%)	603 (97%)	19 (3%)	0	100	100
1	C	629/707 (89%)	609 (97%)	20 (3%)	0	100	100
1	D	624/707 (88%)	610 (98%)	14 (2%)	0	100	100
All	All	2506/2828 (89%)	2438 (97%)	67 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ALA

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	543/592 (92%)	516 (95%)	27 (5%)	24	30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	538/592 (91%)	522 (97%)	16 (3%)	41	53
1	C	539/592 (91%)	516 (96%)	23 (4%)	29	36
1	D	537/592 (91%)	512 (95%)	25 (5%)	26	33
All	All	2157/2368 (91%)	2066 (96%)	91 (4%)	30	38

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	57	GLN
1	A	59	ARG
1	A	84	THR
1	A	92	ARG
1	A	94	THR
1	A	102	GLU
1	A	107	CYS
1	A	115	LYS
1	A	162	ASN
1	A	166	LYS
1	A	179	LEU
1	A	202	ASP
1	A	209	GLU
1	A	233	THR
1	A	253	LEU
1	A	268	ARG
1	A	353	ASN
1	A	364	ARG
1	A	374	SER
1	A	528	LEU
1	A	562	THR
1	A	568	LYS
1	A	575	ASP
1	A	672	CYS
1	A	673	LEU
1	A	674	GLN
1	B	43	LEU
1	B	59	ARG
1	B	94	THR
1	B	102	GLU
1	B	107	CYS
1	B	179	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	233	THR
1	B	268	ARG
1	B	312	ASP
1	B	374	SER
1	B	392	LYS
1	B	528	LEU
1	B	562	THR
1	B	605	LYS
1	B	618	VAL
1	B	673	LEU
1	C	26	LYS
1	C	43	LEU
1	C	56	GLU
1	C	92	ARG
1	C	94	THR
1	C	98	SER
1	C	102	GLU
1	C	107	CYS
1	C	179	LEU
1	C	233	THR
1	C	268	ARG
1	C	275	LEU
1	C	298	SER
1	C	353	ASN
1	C	363	ASP
1	C	392	LYS
1	C	459	GLN
1	C	528	LEU
1	C	552	LEU
1	C	562	THR
1	C	619	ARG
1	C	673	LEU
1	C	677	LEU
1	D	43	LEU
1	D	59	ARG
1	D	92	ARG
1	D	94	THR
1	D	102	GLU
1	D	107	CYS
1	D	150	GLU
1	D	179	LEU
1	D	209	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	222	GLN
1	D	233	THR
1	D	268	ARG
1	D	312	ASP
1	D	324	LEU
1	D	353	ASN
1	D	363	ASP
1	D	528	LEU
1	D	552	LEU
1	D	562	THR
1	D	568	LYS
1	D	576	THR
1	D	580	ARG
1	D	599	VAL
1	D	670	LEU
1	D	673	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	GLN
1	D	674	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	641/707 (90%)	0.47	42 (6%) 18 17	20, 37, 61, 92	0
1	B	636/707 (89%)	0.44	39 (6%) 21 20	20, 40, 66, 81	0
1	C	639/707 (90%)	0.48	51 (7%) 12 11	19, 39, 72, 93	0
1	D	636/707 (89%)	0.49	39 (6%) 21 20	20, 39, 64, 85	0
All	All	2552/2828 (90%)	0.47	171 (6%) 17 16	19, 39, 66, 93	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	276	ILE	6.9
1	C	279	VAL	6.8
1	C	275	LEU	6.3
1	C	369	ALA	5.2
1	B	276	ILE	5.2
1	C	278	LYS	4.7
1	C	281	PRO	4.5
1	C	277	HIS	4.2
1	A	86	PHE	3.9
1	B	564	LEU	3.8
1	D	279	VAL	3.8
1	C	579	ASP	3.8
1	A	276	ILE	3.7
1	A	275	LEU	3.7
1	B	522	ASN	3.6
1	D	568	LYS	3.6
1	C	443	LEU	3.6
1	A	32	THR	3.5
1	C	57	GLN	3.5
1	C	451	VAL	3.5
1	A	363	ASP	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	590	ASP	3.3
1	A	444	ALA	3.3
1	D	577	LEU	3.3
1	C	280	LYS	3.2
1	C	583	GLU	3.2
1	B	284	GLY	3.2
1	D	360	HIS	3.1
1	B	584	PHE	3.1
1	A	57	GLN	3.1
1	B	565	ALA	3.1
1	C	282	HIS	3.1
1	B	562	THR	3.1
1	D	440	LEU	3.1
1	C	440	LEU	3.0
1	C	56	GLU	3.0
1	D	369	ALA	3.0
1	C	591	ARG	3.0
1	D	366	LEU	3.0
1	A	587	ARG	2.9
1	B	449	THR	2.9
1	C	447	VAL	2.9
1	B	443	LEU	2.9
1	B	510	VAL	2.9
1	D	442	TYR	2.9
1	B	529	LEU	2.9
1	C	588	LEU	2.9
1	D	443	LEU	2.9
1	A	359	ASP	2.8
1	A	443	LEU	2.8
1	B	451	VAL	2.8
1	D	75	ASP	2.8
1	A	364	ARG	2.8
1	C	585	GLU	2.8
1	A	373	GLY	2.8
1	C	514	LEU	2.8
1	A	358	ILE	2.8
1	C	285	GLN	2.7
1	C	567	HIS	2.7
1	B	523	ASP	2.7
1	D	71	ARG	2.7
1	C	442	TYR	2.7
1	A	385	ILE	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	444	ALA	2.7
1	C	61	ARG	2.7
1	C	175	ALA	2.7
1	D	175	ALA	2.7
1	D	62	VAL	2.6
1	D	215	GLY	2.6
1	C	587	ARG	2.6
1	A	584	PHE	2.6
1	B	444	ALA	2.6
1	B	586	LYS	2.6
1	A	591	ARG	2.6
1	C	559	CYS	2.6
1	B	588	LEU	2.6
1	B	447	VAL	2.6
1	B	508	GLU	2.6
1	A	581	LEU	2.6
1	C	438	SER	2.5
1	B	442	TYR	2.5
1	D	576	THR	2.5
1	D	567	HIS	2.5
1	B	674	GLN	2.5
1	C	385	ILE	2.5
1	A	552	LEU	2.5
1	D	447	VAL	2.5
1	D	208	PRO	2.5
1	A	395	PHE	2.5
1	D	675	GLY	2.5
1	D	387	VAL	2.5
1	D	448	THR	2.5
1	D	367	HIS	2.5
1	D	202	ASP	2.5
1	A	279	VAL	2.5
1	B	461	ILE	2.4
1	B	524	THR	2.4
1	D	673	LEU	2.4
1	A	448	THR	2.4
1	A	367	HIS	2.4
1	A	394	LEU	2.4
1	B	566	LEU	2.4
1	C	646	GLU	2.4
1	C	58	CYS	2.4
1	C	446	PRO	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	526	ALA	2.4
1	D	449	THR	2.4
1	D	65	CYS	2.4
1	C	581	LEU	2.4
1	D	451	VAL	2.4
1	C	444	ALA	2.4
1	C	449	THR	2.4
1	B	518	CYS	2.3
1	B	446	PRO	2.3
1	C	388	ALA	2.3
1	B	576	THR	2.3
1	B	199	ILE	2.3
1	A	579	ASP	2.3
1	A	524	THR	2.3
1	C	564	LEU	2.3
1	A	121	VAL	2.3
1	C	586	LYS	2.3
1	C	450	HIS	2.3
1	D	383	VAL	2.3
1	B	448	THR	2.3
1	B	521	PRO	2.3
1	B	563	ILE	2.3
1	A	442	TYR	2.2
1	B	454	ALA	2.2
1	C	584	PHE	2.2
1	B	559	CYS	2.2
1	C	560	PHE	2.2
1	D	630	ARG	2.2
1	D	676	PHE	2.2
1	B	285	GLN	2.2
1	A	586	LYS	2.2
1	D	76	GLY	2.2
1	B	440	LEU	2.2
1	B	464	LEU	2.2
1	A	389	GLY	2.2
1	A	449	THR	2.2
1	D	211	LEU	2.2
1	D	437	SER	2.2
1	B	47	HIS	2.2
1	C	605	LYS	2.2
1	A	578	VAL	2.2
1	C	286	ILE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	276	ILE	2.1
1	C	464	LEU	2.1
1	A	507	VAL	2.1
1	A	284	GLY	2.1
1	C	434	ALA	2.1
1	B	203	VAL	2.1
1	A	446	PRO	2.1
1	A	366	LEU	2.1
1	A	440	LEU	2.1
1	B	581	LEU	2.1
1	A	523	ASP	2.1
1	D	203	VAL	2.1
1	C	448	THR	2.1
1	B	277	HIS	2.1
1	A	217	ARG	2.0
1	A	393	LEU	2.0
1	C	592	LEU	2.0
1	D	579	ASP	2.0
1	D	459	GLN	2.0
1	C	582	ALA	2.0
1	D	201	ASP	2.0
1	A	566	LEU	2.0
1	C	541	LEU	2.0
1	A	387	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 monosaccharides 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.