



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:20 PM GMT

PDB ID : 4C6G  
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 : 2013-09-18  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
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

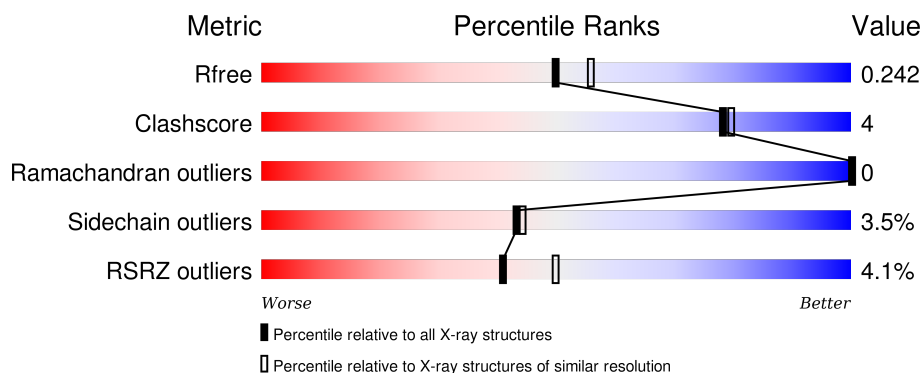
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	707	<div> <div>5%</div> <div>80% 8% • 12%</div> </div>
1	B	707	<div> <div>4%</div> <div>78% 10% • 11%</div> </div>
1	C	707	<div> <div>4%</div> <div>78% 10% • 12%</div> </div>
1	D	707	<div> <div>2%</div> <div>77% 11% • 11%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19587 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	624	Total	C	N	O	S	0	0	0
			4833	3074	826	911	22			
1	B	626	Total	C	N	O	S	0	0	0
			4848	3085	828	913	22			
1	C	625	Total	C	N	O	S	0	0	0
			4839	3078	825	914	22			
1	D	626	Total	C	N	O	S	0	0	0
			4847	3083	828	914	22			

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	231	ALA	ASN	ENGINEERED MUTATION	UNP Q68G84

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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	231	ALA	ASN	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	231	ALA	ASN	ENGINEERED MUTATION	UNP Q68G84

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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	231	ALA	ASN	ENGINEERED MUTATION	UNP Q68G84

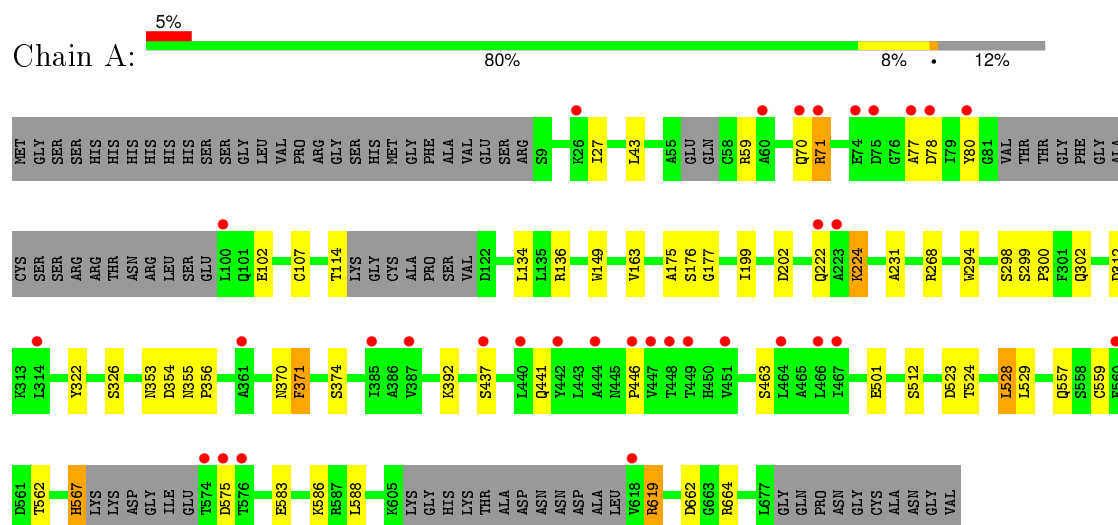
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	73	Total O 73 73	0	0
2	B	42	Total O 42 42	0	0
2	C	60	Total O 60 60	0	0
2	D	45	Total O 45 45	0	0

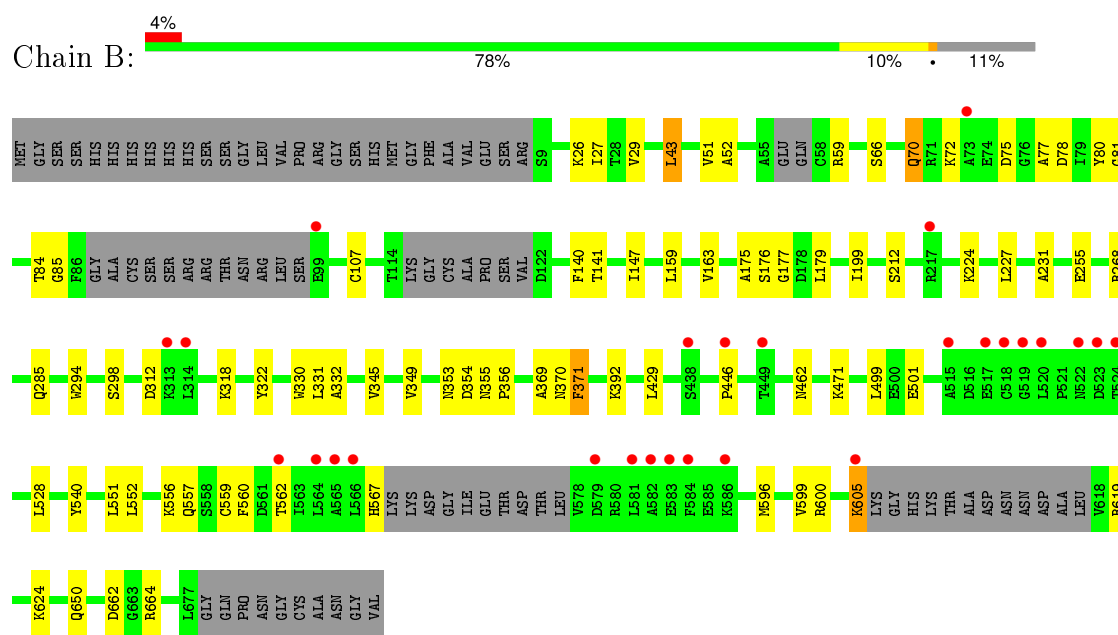
### 3 Residue-property plots [i](#)

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.

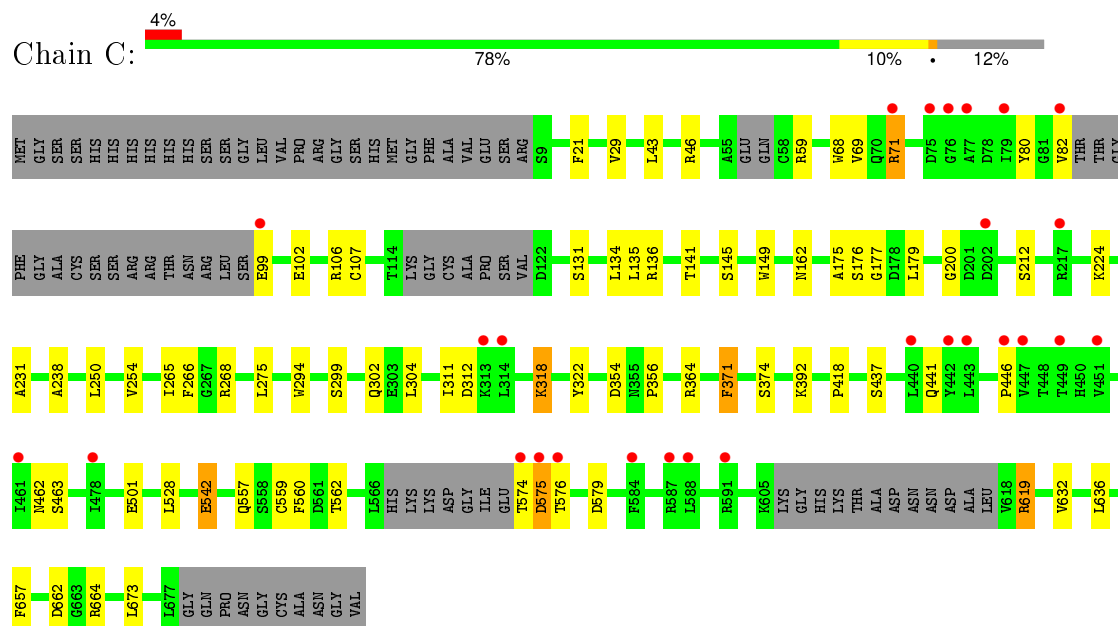
#### • Molecule 1: PHENYLALANINE AMMONIA-LYASE



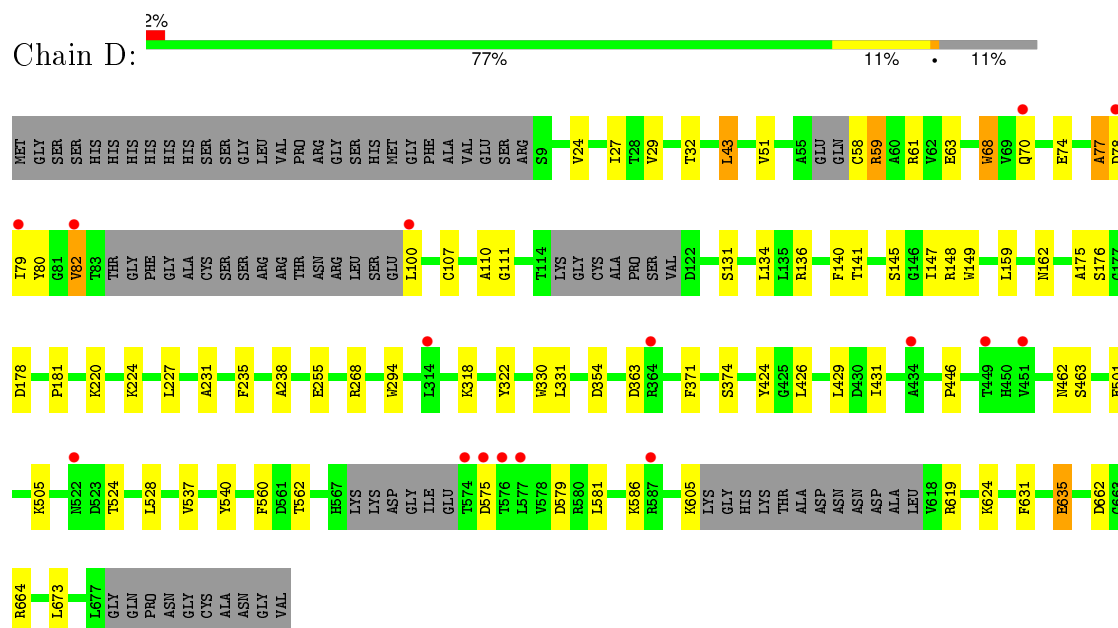
#### • Molecule 1: PHENYLALANINE AMMONIA-LYASE



#### • 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, $\alpha$ , $\beta$ , $\gamma$	98.96Å 146.57Å 99.33Å 90.00° 100.02° 90.00°	Depositor
Resolution (Å)	48.73 – 2.10 48.08 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.73-2.10) 99.7 (48.08-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.201 , 0.241 0.203 , 0.242	Depositor DCC
$R_{free}$ test set	8119 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.2	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.1	EDS
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 161768 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.61	5/4916 (0.1%)	0.68	8/6671 (0.1%)
1	B	0.60	4/4932 (0.1%)	0.65	4/6692 (0.1%)
1	C	0.64	7/4921 (0.1%)	0.76	2/6678 (0.0%)
1	D	0.63	6/4930 (0.1%)	0.65	4/6691 (0.1%)
All	All	0.62	22/19699 (0.1%)	0.68	18/26732 (0.1%)

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	C	0	1
1	D	0	1
All	All	0	2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	71	ARG	CZ-NH2	20.26	1.59	1.33
1	D	77	ALA	C-N	-19.91	0.88	1.34
1	A	77	ALA	C-N	-19.16	0.90	1.34
1	B	77	ALA	C-N	-18.35	0.91	1.34
1	C	71	ARG	CZ-NH1	-15.19	1.13	1.33
1	D	78	ASP	C-N	-13.28	1.03	1.34
1	B	78	ASP	C-N	-12.47	1.05	1.34
1	A	78	ASP	C-N	-10.42	1.10	1.34
1	C	71	ARG	NE-CZ	6.67	1.41	1.33
1	B	330	TRP	CD2-CE2	5.52	1.48	1.41
1	C	71	ARG	CD-NE	5.48	1.55	1.46
1	D	330	TRP	CD2-CE2	5.45	1.47	1.41
1	C	149	TRP	CD2-CE2	5.35	1.47	1.41
1	D	68	TRP	CD2-CE2	5.29	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	294	TRP	CD2-CE2	5.26	1.47	1.41
1	B	294	TRP	CD2-CE2	5.18	1.47	1.41
1	C	294	TRP	CD2-CE2	5.18	1.47	1.41
1	C	68	TRP	CD2-CE2	5.17	1.47	1.41
1	D	294	TRP	CD2-CE2	5.14	1.47	1.41
1	A	71	ARG	CZ-NH2	5.12	1.39	1.33
1	D	149	TRP	CD2-CE2	5.07	1.47	1.41
1	A	149	TRP	CD2-CE2	5.04	1.47	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	71	ARG	NE-CZ-NH2	-31.23	104.69	120.30
1	C	71	ARG	NE-CZ-NH1	14.93	127.77	120.30
1	A	71	ARG	NE-CZ-NH2	-14.50	113.05	120.30
1	B	77	ALA	O-C-N	-11.49	104.32	122.70
1	D	78	ASP	O-C-N	-11.29	104.63	122.70
1	A	77	ALA	O-C-N	-9.00	108.29	122.70
1	B	77	ALA	C-N-CA	7.93	141.51	121.70
1	A	78	ASP	O-C-N	-7.89	110.08	122.70
1	D	78	ASP	CA-C-N	7.87	134.50	117.20
1	B	77	ALA	CA-C-N	7.83	134.43	117.20
1	A	77	ALA	C-N-CA	7.73	141.02	121.70
1	A	77	ALA	CA-C-N	5.91	130.20	117.20
1	A	78	ASP	C-N-CA	5.51	135.46	121.70
1	D	78	ASP	C-N-CA	5.46	135.36	121.70
1	B	78	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	78	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	78	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	78	ASP	CA-C-N	5.06	128.33	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	71	ARG	Sidechain
1	D	77	ALA	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4833	0	4901	29	0
1	B	4848	0	4913	47	0
1	C	4839	0	4911	50	0
1	D	4847	0	4917	42	0
2	A	73	0	0	0	0
2	B	42	0	0	0	0
2	C	60	0	0	0	0
2	D	45	0	0	0	0
All	All	19587	0	19642	142	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 (142) 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:80:TYR:HB3	1:B:318:LYS:HG2	1.58	0.85
1:C:80:TYR:CB	1:D:318:LYS:HG2	2.09	0.81
1:C:304:LEU:HD11	1:C:619:ARG:HD3	1.64	0.80
1:A:80:TYR:CB	1:B:318:LYS:HG2	2.11	0.80
1:C:80:TYR:HB3	1:D:318:LYS:HG2	1.67	0.77
1:C:501:GLU:OE1	1:C:619:ARG:HD2	1.86	0.74
1:C:99:GLU:HA	1:C:102:GLU:HG2	1.76	0.67
1:B:552:LEU:O	1:B:556:LYS:HG3	1.94	0.66
1:C:574:THR:HG23	1:C:575:ASP:N	2.11	0.66
1:D:70:GLN:O	1:D:74:GLU:HG2	1.98	0.64
1:A:662:ASP:OD1	1:A:664:ARG:HD3	1.99	0.63
1:A:176:SER:HB3	1:B:322:TYR:OH	1.99	0.62
1:C:176:SER:HB3	1:D:322:TYR:OH	2.00	0.61
1:C:418:PRO:O	1:C:542:GLU:HB2	2.00	0.61
1:C:318:LYS:HG2	1:D:80:TYR:HB2	1.82	0.61
1:C:322:TYR:OH	1:D:176:SER:HB3	2.00	0.60
1:C:162:ASN:HD22	1:C:200:GLY:HA2	1.68	0.57
1:D:255:GLU:HG2	1:D:331:LEU:HD13	1.86	0.57
1:D:231:ALA:O	1:D:354:ASP:HA	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LEU:HD22	1:A:134:LEU:HD22	1.87	0.56
1:B:231:ALA:HB1	1:B:371:PHE:HD2	1.70	0.56
1:B:557:GLN:OE1	1:C:557:GLN:NE2	2.37	0.56
1:C:446:PRO:HD3	1:D:446:PRO:HD3	1.88	0.55
1:C:574:THR:HG23	1:C:575:ASP:H	1.71	0.55
1:B:27:ILE:CD1	1:B:43:LEU:HB2	2.36	0.55
1:D:131:SER:HB2	1:D:238:ALA:HB1	1.89	0.55
1:D:43:LEU:HD22	1:D:134:LEU:HD22	1.89	0.55
1:C:318:LYS:HG2	1:D:80:TYR:CB	2.37	0.55
1:C:437:SER:O	1:C:441:GLN:HG2	2.07	0.54
1:B:224:LYS:HE2	1:B:356:PRO:HD2	1.88	0.54
1:A:175:ALA:C	1:A:177:GLY:H	2.11	0.54
1:A:114:THR:HG22	1:C:657:PHE:CZ	2.43	0.53
1:A:70:GLN:OE1	1:A:222:GLN:HB3	2.09	0.52
1:A:231:ALA:O	1:A:354:ASP:HA	2.09	0.52
1:B:501:GLU:OE2	1:B:619:ARG:NH1	2.42	0.52
1:B:429:LEU:HD23	1:D:110:ALA:HB1	1.91	0.52
1:D:58:CYS:HA	1:D:61:ARG:HE	1.74	0.51
1:C:574:THR:CG2	1:C:575:ASP:N	2.73	0.51
1:B:85:GLY:HA2	1:D:424:TYR:OH	2.10	0.51
1:B:560:PHE:CE1	1:C:559:CYS:HB3	2.45	0.51
1:D:145:SER:O	1:D:224:LYS:HD3	2.11	0.51
1:C:231:ALA:O	1:C:354:ASP:HA	2.11	0.51
1:A:446:PRO:HD3	1:B:446:PRO:HD3	1.93	0.51
1:B:80:TYR:HA	1:B:84:THR:HB	1.93	0.50
1:C:224:LYS:HE2	1:C:356:PRO:HD2	1.93	0.50
1:B:179:LEU:HD12	1:D:431:ILE:HD13	1.93	0.50
1:B:231:ALA:HB1	1:B:371:PHE:CD2	2.46	0.50
1:B:29:VAL:HG12	1:B:141:THR:HG21	1.94	0.50
1:D:29:VAL:HG12	1:D:141:THR:HG21	1.93	0.50
1:D:51:VAL:HG21	1:D:159:LEU:HD13	1.93	0.50
1:B:567:HIS:CE1	1:C:575:ASP:OD1	2.65	0.49
1:C:574:THR:CG2	1:C:575:ASP:H	2.25	0.49
1:D:524:THR:HG21	1:D:581:LEU:HD21	1.94	0.49
1:B:559:CYS:O	1:B:562:THR:HG22	2.12	0.49
1:B:559:CYS:HB3	1:C:560:PHE:CE1	2.47	0.49
1:D:374:SER:HA	1:D:463:SER:HB2	1.95	0.48
1:A:322:TYR:OH	1:B:176:SER:HB3	2.13	0.48
1:C:175:ALA:HB2	1:C:462:ASN:HB2	1.95	0.48
1:A:501:GLU:OE1	1:A:619:ARG:HD2	2.13	0.48
1:C:299:SER:HB3	1:C:302:GLN:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:THR:HG22	1:A:528:LEU:HD22	1.95	0.48
1:C:162:ASN:ND2	1:C:200:GLY:HA2	2.29	0.47
1:B:163:VAL:HG22	1:B:199:ILE:HG12	1.97	0.47
1:C:250:LEU:O	1:C:254:VAL:HG23	2.15	0.47
1:D:175:ALA:HB2	1:D:462:ASN:CB	2.44	0.47
1:A:163:VAL:HG22	1:A:199:ILE:HG12	1.97	0.47
1:D:524:THR:HG23	1:D:562:THR:HG21	1.95	0.47
1:C:69:VAL:HG13	1:C:82:VAL:HG13	1.97	0.46
1:A:224:LYS:HE3	1:A:356:PRO:HD2	1.98	0.46
1:B:560:PHE:HB2	1:C:560:PHE:HB2	1.96	0.46
1:D:68:TRP:HE1	1:D:363:ASP:HA	1.79	0.46
1:C:80:TYR:CG	1:D:318:LYS:HG2	2.49	0.46
1:D:175:ALA:HB2	1:D:462:ASN:HB2	1.98	0.46
1:B:355:ASN:HB3	1:B:371:PHE:CE2	2.50	0.46
1:B:51:VAL:HG21	1:B:159:LEU:HD13	1.97	0.46
1:C:304:LEU:CD1	1:C:619:ARG:HD3	2.39	0.45
1:B:650:GLN:HG3	1:D:111:GLY:O	2.16	0.45
1:A:231:ALA:HB1	1:A:371:PHE:HD2	1.82	0.45
1:B:596:MET:O	1:B:599:VAL:HG12	2.16	0.45
1:C:99:GLU:HA	1:C:102:GLU:CG	2.42	0.45
1:C:576:THR:HA	1:C:579:ASP:HB2	1.99	0.45
1:A:353:ASN:HA	1:A:370:ASN:HB3	1.99	0.45
1:C:224:LYS:HG2	1:C:224:LYS:O	2.16	0.45
1:C:374:SER:HA	1:C:463:SER:HB2	1.99	0.45
1:C:145:SER:O	1:C:224:LYS:HD3	2.17	0.45
1:A:559:CYS:HB3	1:D:560:PHE:CE1	2.52	0.44
1:B:605:LYS:HE2	1:B:605:LYS:HB3	1.58	0.44
1:C:175:ALA:C	1:C:177:GLY:H	2.19	0.44
1:C:29:VAL:HG12	1:C:141:THR:HG21	1.99	0.44
1:B:255:GLU:HG2	1:B:331:LEU:HD13	1.99	0.44
1:B:175:ALA:HB2	1:B:462:ASN:CB	2.48	0.44
1:D:426:LEU:HG	1:D:429:LEU:HD12	1.99	0.44
1:B:81:GLY:HA3	1:B:227:LEU:HD22	1.99	0.44
1:A:355:ASN:HB3	1:A:371:PHE:CE2	2.53	0.44
1:D:181:PRO:HB2	1:D:235:PHE:CD2	2.52	0.44
1:C:632:VAL:HA	1:C:636:LEU:HD12	2.00	0.44
1:B:345:VAL:O	1:B:349:VAL:HG23	2.17	0.43
1:D:501:GLU:OE1	1:D:619:ARG:HD2	2.18	0.43
1:A:567:HIS:CE1	1:D:579:ASP:OD1	2.71	0.43
1:B:175:ALA:HB2	1:B:462:ASN:HB2	1.98	0.43
1:D:79:ILE:HG22	1:D:82:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ARG:NH2	1:D:220:LYS:O	2.51	0.43
1:A:374:SER:HA	1:A:463:SER:HB2	2.00	0.43
1:A:299:SER:HA	1:A:300:PRO:HD2	1.87	0.43
1:B:175:ALA:C	1:B:177:GLY:H	2.21	0.43
1:C:131:SER:HB3	1:C:238:ALA:HB1	2.00	0.43
1:B:231:ALA:O	1:B:354:ASP:HA	2.19	0.42
1:C:175:ALA:HB2	1:C:462:ASN:CB	2.49	0.42
1:A:202:ASP:N	1:A:202:ASP:OD1	2.52	0.42
1:C:176:SER:HA	1:C:371:PHE:CD1	2.54	0.42
1:D:59:ARG:NH1	1:D:63:GLU:OE2	2.43	0.42
1:C:43:LEU:HD13	1:C:134:LEU:HD22	2.01	0.42
1:B:72:LYS:HD3	1:B:72:LYS:HA	1.89	0.42
1:B:84:THR:HG22	1:B:85:GLY:O	2.20	0.42
1:A:512:SER:HB2	1:A:529:LEU:HD21	2.00	0.42
1:D:537:VAL:HA	1:D:540:TYR:CE2	2.54	0.42
1:C:662:ASP:OD1	1:C:664:ARG:HD3	2.19	0.42
1:A:27:ILE:CD1	1:A:43:LEU:HB2	2.49	0.42
1:D:318:LYS:O	1:D:318:LYS:HG3	2.19	0.42
1:A:588:LEU:HA	1:A:588:LEU:HD12	1.92	0.42
1:D:140:PHE:CG	1:D:147:ILE:HG21	2.54	0.42
1:B:471:LYS:HD3	1:B:471:LYS:HA	1.84	0.42
1:B:540:TYR:CE1	1:B:551:LEU:HD22	2.55	0.42
1:C:265:ILE:O	1:C:266:PHE:HB2	2.19	0.42
1:B:66:SER:O	1:B:70:GLN:NE2	2.53	0.42
1:A:437:SER:O	1:A:441:GLN:HG2	2.20	0.41
1:C:224:LYS:NZ	1:C:354:ASP:OD2	2.54	0.41
1:D:178:ASP:HB3	1:D:181:PRO:HG2	2.03	0.41
1:C:21:PHE:O	1:C:46:ARG:NH1	2.53	0.41
1:D:631:PHE:O	1:D:635:GLU:HB2	2.21	0.41
1:D:27:ILE:CD1	1:D:43:LEU:HB2	2.51	0.41
1:B:662:ASP:OD1	1:B:664:ARG:HD3	2.21	0.41
1:A:299:SER:HB3	1:A:302:GLN:HG2	2.03	0.41
1:D:662:ASP:OD1	1:D:664:ARG:HD3	2.21	0.40
1:B:285:GLN:HB2	1:B:332:ALA:HB2	2.03	0.40
1:A:326:SER:HB3	1:B:369:ALA:CB	2.51	0.40
1:B:353:ASN:HA	1:B:370:ASN:HB3	2.04	0.40
1:C:99:GLU:HA	1:C:102:GLU:OE2	2.22	0.40
1:C:176:SER:OG	1:C:179:LEU:HD11	2.22	0.40
1:B:26:LYS:HE2	1:B:52:ALA:HB2	2.04	0.40
1:B:499:LEU:HD21	1:B:600:ARG:HG3	2.03	0.40
1:B:140:PHE:CG	1:B:147:ILE:HG21	2.57	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	612/707 (87%)	596 (97%)	16 (3%)	0	100	100
1	B	614/707 (87%)	592 (96%)	22 (4%)	0	100	100
1	C	613/707 (87%)	598 (98%)	15 (2%)	0	100	100
1	D	614/707 (87%)	597 (97%)	17 (3%)	0	100	100
All	All	2453/2828 (87%)	2383 (97%)	70 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	527/592 (89%)	507 (96%)	20 (4%)	40	40
1	B	528/592 (89%)	514 (97%)	14 (3%)	52	56
1	C	528/592 (89%)	508 (96%)	20 (4%)	40	40
1	D	529/592 (89%)	509 (96%)	20 (4%)	40	40
All	All	2112/2368 (89%)	2038 (96%)	74 (4%)	43	44

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	71	ARG
1	A	102	GLU
1	A	107	CYS
1	A	136	ARG
1	A	224	LYS
1	A	268	ARG
1	A	298	SER
1	A	312	ASP
1	A	371	PHE
1	A	392	LYS
1	A	523	ASP
1	A	528	LEU
1	A	557	GLN
1	A	562	THR
1	A	567	HIS
1	A	575	ASP
1	A	583	GLU
1	A	586	LYS
1	A	619	ARG
1	B	43	LEU
1	B	59	ARG
1	B	70	GLN
1	B	75	ASP
1	B	107	CYS
1	B	212	SER
1	B	268	ARG
1	B	298	SER
1	B	312	ASP
1	B	371	PHE
1	B	392	LYS
1	B	528	LEU
1	B	605	LYS
1	B	624	LYS
1	C	59	ARG
1	C	106	ARG
1	C	107	CYS
1	C	135	LEU
1	C	136	ARG
1	C	212	SER
1	C	268	ARG
1	C	275	LEU
1	C	311	ILE

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Mol	Chain	Res	Type
1	C	312	ASP
1	C	318	LYS
1	C	364	ARG
1	C	371	PHE
1	C	392	LYS
1	C	528	LEU
1	C	542	GLU
1	C	562	THR
1	C	575	ASP
1	C	619	ARG
1	C	673	LEU
1	D	24	VAL
1	D	32	THR
1	D	43	LEU
1	D	59	ARG
1	D	82	VAL
1	D	100	LEU
1	D	107	CYS
1	D	136	ARG
1	D	162	ASN
1	D	227	LEU
1	D	268	ARG
1	D	371	PHE
1	D	505	LYS
1	D	528	LEU
1	D	575	ASP
1	D	586	LYS
1	D	605	LYS
1	D	624	LYS
1	D	635	GLU
1	D	673	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	557	GLN
1	A	567	HIS
1	B	557	GLN
1	C	557	GLN
1	D	557	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	624/707 (88%)	0.23	33 (5%) 30 39	27, 43, 66, 99	0
1	B	626/707 (88%)	0.21	27 (4%) 39 48	26, 45, 69, 91	0
1	C	625/707 (88%)	0.18	27 (4%) 39 48	27, 43, 68, 95	0
1	D	626/707 (88%)	0.24	16 (2%) 59 66	27, 43, 64, 81	0
All	All	2501/2828 (88%)	0.22	103 (4%) 41 50	26, 44, 67, 99	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	LEU	6.8
1	C	314	LEU	5.6
1	D	314	LEU	4.9
1	B	99	GLU	3.9
1	D	576	THR	3.8
1	A	574	THR	3.7
1	D	78	ASP	3.7
1	B	564	LEU	3.6
1	D	574	THR	3.5
1	B	217	ARG	3.4
1	C	202	ASP	3.3
1	B	584	PHE	3.3
1	C	82	VAL	3.2
1	A	314	LEU	3.2
1	D	79	ILE	3.2
1	A	447	VAL	3.2
1	A	70	GLN	3.1
1	A	361	ALA	3.1
1	D	451	VAL	3.0
1	B	313	LYS	3.0
1	A	77	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	566	LEU	3.0
1	B	579	ASP	3.0
1	A	71	ARG	3.0
1	C	591	ARG	2.9
1	D	577	LEU	2.8
1	B	565	ALA	2.8
1	B	524	THR	2.8
1	B	581	LEU	2.8
1	C	76	GLY	2.8
1	C	313	LYS	2.8
1	A	464	LEU	2.8
1	C	576	THR	2.8
1	A	75	ASP	2.8
1	D	522	ASN	2.8
1	A	467	ILE	2.8
1	D	575	ASP	2.7
1	C	588	LEU	2.7
1	C	574	THR	2.7
1	C	443	LEU	2.7
1	C	71	ARG	2.7
1	C	217	ARG	2.7
1	D	587	ARG	2.7
1	B	586	LYS	2.7
1	D	70	GLN	2.6
1	A	449	THR	2.6
1	B	449	THR	2.6
1	A	222	GLN	2.6
1	A	74	GLU	2.5
1	A	223	ALA	2.5
1	D	100	LEU	2.5
1	A	451	VAL	2.5
1	B	583	GLU	2.5
1	D	449	THR	2.5
1	A	78	ASP	2.5
1	B	582	ALA	2.5
1	C	451	VAL	2.5
1	C	575	ASP	2.4
1	A	444	ALA	2.4
1	B	522	ASN	2.4
1	A	446	PRO	2.4
1	C	75	ASP	2.4
1	B	519	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	515	ALA	2.4
1	D	82	VAL	2.4
1	B	517	GLU	2.4
1	A	575	ASP	2.3
1	B	523	ASP	2.3
1	A	385	ILE	2.3
1	A	466	LEU	2.3
1	A	448	THR	2.3
1	A	26	LYS	2.3
1	A	437	SER	2.3
1	B	518	CYS	2.3
1	C	79	ILE	2.3
1	C	449	THR	2.3
1	A	60	ALA	2.3
1	B	520	LEU	2.3
1	A	442	TYR	2.3
1	A	80	TYR	2.2
1	C	99	GLU	2.2
1	B	73	ALA	2.2
1	A	440	LEU	2.2
1	B	446	PRO	2.2
1	A	387	VAL	2.2
1	A	618	VAL	2.2
1	D	434	ALA	2.2
1	C	446	PRO	2.1
1	C	587	ARG	2.1
1	D	364	ARG	2.1
1	A	576	THR	2.1
1	C	77	ALA	2.1
1	B	605	LYS	2.1
1	C	478	ILE	2.1
1	A	100	LEU	2.1
1	C	440	LEU	2.1
1	B	562	THR	2.1
1	A	560	PHE	2.1
1	C	447	VAL	2.1
1	C	461	ILE	2.0
1	C	442	TYR	2.0
1	B	438	SER	2.0
1	C	584	PHE	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.