



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:10 pm BST

PDB ID : 3HJ6  
Title : Structure of Halothermothrix orenii fructokinase (FRK)  
Authors : Chua, T.K.; Seetharaman, J.; Kasprzak, J.M.; Ng, C.; Patel, B.K.; Love, C.;  
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Deposited on : 2009-05-21  
Resolution : 2.80 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

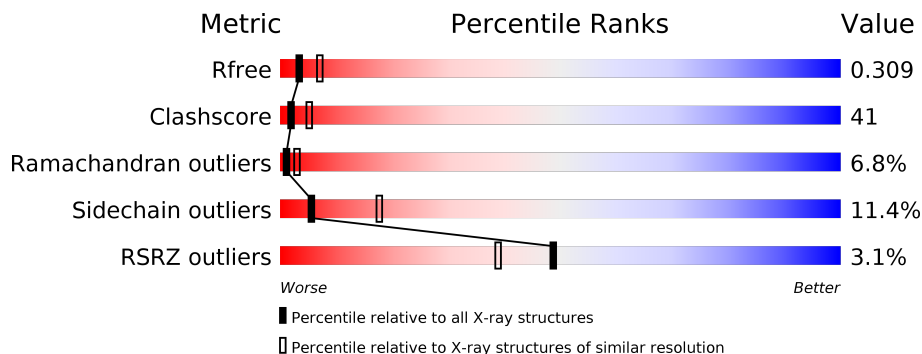
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	327	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 46%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">4%      46%      29%      9%      •      15%</p>
1	B	327	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 43%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 34%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">%      43%      34%      7%      •      15%</p>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4079 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 Fructokinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	278	1968	1242	341	380	3	2	0	0	0
1	B	278	1969	1243	341	380	3	2	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	SEE REMARK 999	UNP B8CZ52
A	2	LYS	-	SEE REMARK 999	UNP B8CZ52
A	3	GLY	-	SEE REMARK 999	UNP B8CZ52
A	4	GLU	-	SEE REMARK 999	UNP B8CZ52
A	5	GLY	-	SEE REMARK 999	UNP B8CZ52
A	6	VAL	-	SEE REMARK 999	UNP B8CZ52
A	7	ILE	-	SEE REMARK 999	UNP B8CZ52
A	8	VAL	-	SEE REMARK 999	UNP B8CZ52
B	1	MSE	-	SEE REMARK 999	UNP B8CZ52
B	2	LYS	-	SEE REMARK 999	UNP B8CZ52
B	3	GLY	-	SEE REMARK 999	UNP B8CZ52
B	4	GLU	-	SEE REMARK 999	UNP B8CZ52
B	5	GLY	-	SEE REMARK 999	UNP B8CZ52
B	6	VAL	-	SEE REMARK 999	UNP B8CZ52
B	7	ILE	-	SEE REMARK 999	UNP B8CZ52
B	8	VAL	-	SEE REMARK 999	UNP B8CZ52

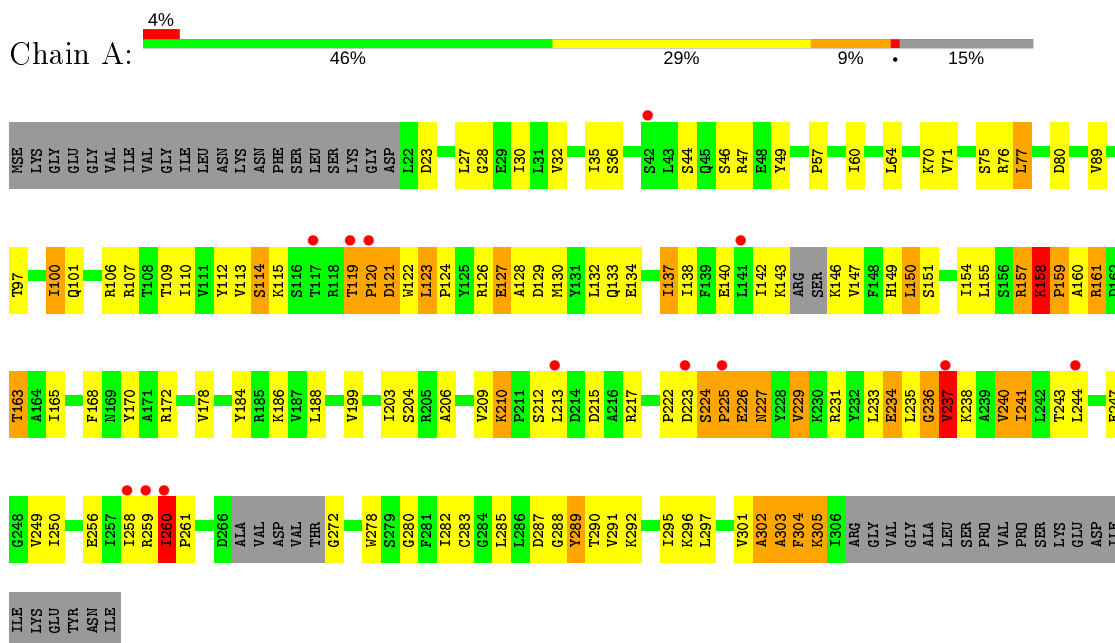
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	56	Total	O	0	0
			56	56		
2	B	86	Total	O	0	0
			86	86		

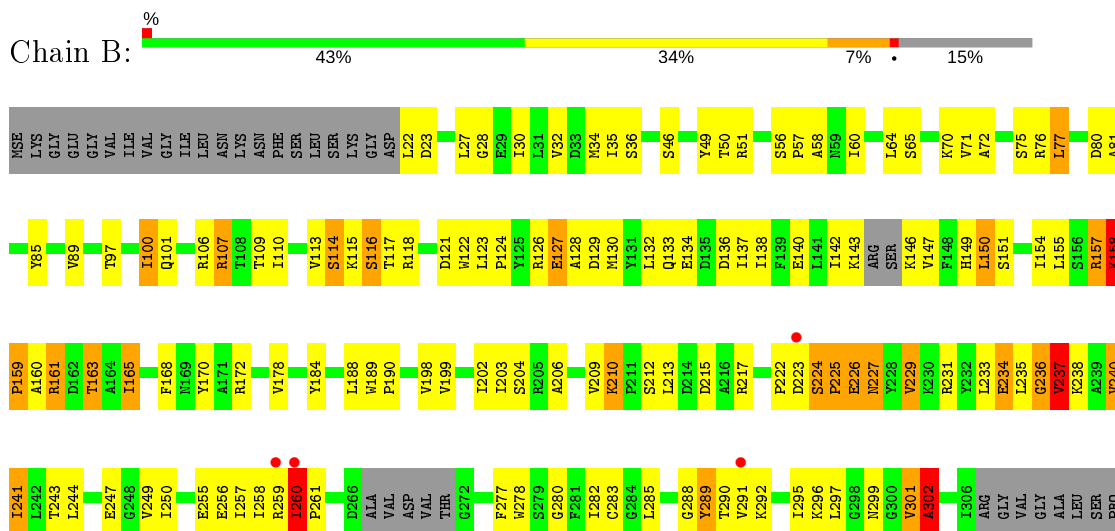
### 3 Residue-property plots

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

- Molecule 1: Fructokinase



- Molecule 1: Fructokinase



VAL  
PRO  
SER  
LYS  
GLU  
ASP  
ILE  
ILE  
LYS  
GLU  
TYR  
ASN  
ILE

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.45Å 171.94Å 46.60Å 90.00° 112.97° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 42.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.5 (50.00-2.80) 97.5 (42.99-2.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.14 (at 2.81Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.254 , 0.288 0.284 , 0.309	Depositor DCC
$R_{free}$ test set	2069 reflections (6.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtrriage
Anisotropy	0.154	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 74.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	4079	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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	0.44	0/1999	0.76	5/2708 (0.2%)
1	B	0.43	0/2000	0.76	4/2710 (0.1%)
All	All	0.44	0/3999	0.76	9/5418 (0.2%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ASP	N-CA-C	-7.48	90.81	111.00
1	A	303	ALA	N-CA-C	6.75	129.24	111.00
1	B	118	ARG	N-CA-C	-6.60	93.17	111.00
1	B	260	ILE	C-N-CD	5.53	140.01	128.40
1	A	260	ILE	C-N-CD	5.47	139.88	128.40
1	B	302	ALA	N-CA-C	-5.43	96.33	111.00
1	A	158	LYS	N-CA-C	5.30	125.30	111.00
1	B	158	LYS	N-CA-C	5.22	125.09	111.00
1	A	302	ALA	N-CA-C	-5.04	97.38	111.00

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	1968	0	1800	153	0
1	B	1969	0	1801	166	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	56	0	0	5	0
2	B	86	0	0	15	0
All	All	4079	0	3601	312	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 41.

All (312) 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:B:260:ILE:HG23	1:B:261:PRO:HD2	1.33	1.10
1:B:260:ILE:HG23	1:B:261:PRO:CD	1.83	1.07
1:A:260:ILE:HG23	1:A:261:PRO:CD	1.83	1.06
1:A:260:ILE:HG23	1:A:261:PRO:HD2	1.40	1.03
1:B:136:ASP:HA	2:B:341:HOH:O	1.62	1.00
1:A:259:ARG:HH11	1:A:259:ARG:HB3	1.30	0.96
1:B:259:ARG:HB3	1:B:259:ARG:HH11	1.31	0.94
1:A:249:VAL:HG12	1:A:260:ILE:CG2	2.01	0.91
1:A:259:ARG:HB3	1:A:259:ARG:NH1	1.86	0.91
1:B:130:MSE:O	1:B:159:PRO:HG2	1.73	0.88
1:B:259:ARG:HB3	1:B:259:ARG:NH1	1.88	0.88
1:A:130:MSE:O	1:A:159:PRO:HG2	1.75	0.86
1:B:249:VAL:HG12	1:B:260:ILE:CG2	2.05	0.85
1:A:291:VAL:HA	2:A:352:HOH:O	1.76	0.84
1:B:137:ILE:HG22	1:B:170:TYR:CD2	2.14	0.83
1:A:301:VAL:HG23	1:A:301:VAL:O	1.81	0.81
1:A:249:VAL:HG12	1:A:260:ILE:HG21	1.62	0.80
1:A:137:ILE:HG22	1:A:170:TYR:CD2	2.17	0.80
1:B:249:VAL:HG12	1:B:260:ILE:HG21	1.63	0.79
1:A:132:LEU:O	1:A:163:THR:HG21	1.82	0.79
1:B:132:LEU:O	1:B:163:THR:HG21	1.83	0.77
1:A:124:PRO:O	1:B:107:ARG:NH1	2.18	0.76
1:A:119:THR:O	1:A:120:PRO:O	2.04	0.76
1:B:77:LEU:HG	1:B:100:ILE:HD11	1.68	0.74
1:A:137:ILE:N	1:A:137:ILE:HD12	2.03	0.74
1:B:122:TRP:CZ3	1:B:124:PRO:HG3	2.23	0.74
1:A:235:LEU:O	1:A:237:VAL:N	2.22	0.73
1:A:260:ILE:HG23	1:A:261:PRO:HD3	1.71	0.73
1:B:143:LYS:C	1:B:146:LYS:HA	2.09	0.73
1:A:100:ILE:HD13	1:A:101:GLN:N	2.04	0.73
1:A:143:LYS:C	1:A:146:LYS:HA	2.10	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LEU:O	1:B:237:VAL:N	2.22	0.72
1:A:32:VAL:CG2	1:A:110:ILE:HG12	2.19	0.72
1:B:100:ILE:HD13	1:B:101:GLN:N	2.05	0.71
1:A:77:LEU:HG	1:A:100:ILE:HD11	1.71	0.71
1:B:137:ILE:N	1:B:137:ILE:HD12	2.07	0.70
1:A:233:LEU:C	1:A:235:LEU:H	1.94	0.70
1:A:222:PRO:O	1:A:224:SER:N	2.24	0.70
1:A:241:ILE:HG12	1:A:249:VAL:HG21	1.73	0.70
1:A:249:VAL:H	1:A:260:ILE:CG2	2.04	0.69
1:B:222:PRO:O	1:B:224:SER:N	2.25	0.69
1:A:149:HIS:CD2	1:A:278:TRP:HE1	2.11	0.69
1:B:32:VAL:CG2	1:B:110:ILE:HG12	2.23	0.69
1:B:233:LEU:C	1:B:235:LEU:H	1.96	0.68
1:B:285:LEU:HA	2:B:349:HOH:O	1.93	0.68
1:A:249:VAL:HG12	1:A:260:ILE:HG22	1.75	0.68
1:A:23:ASP:HB2	1:A:70:LYS:O	1.93	0.68
1:A:241:ILE:HD13	1:A:241:ILE:O	1.94	0.68
1:A:244:LEU:HD11	1:A:250:ILE:CG1	2.24	0.68
1:A:225:PRO:O	1:A:226:GLU:HG3	1.94	0.67
1:B:241:ILE:HG12	1:B:249:VAL:HG21	1.76	0.67
1:B:149:HIS:CD2	1:B:278:TRP:HE1	2.12	0.67
1:B:231:ARG:C	1:B:234:GLU:H	1.97	0.67
1:B:97:THR:O	1:B:100:ILE:HG22	1.95	0.67
1:A:122:TRP:CZ3	1:A:124:PRO:HG3	2.30	0.66
1:A:283:CYS:C	1:A:285:LEU:H	1.99	0.66
1:B:23:ASP:HB2	1:B:70:LYS:O	1.95	0.66
1:B:225:PRO:HD2	1:B:227:ASN:ND2	2.10	0.66
1:A:109:THR:HG23	1:A:126:ARG:HA	1.77	0.66
1:A:225:PRO:HD2	1:A:227:ASN:ND2	2.11	0.65
1:B:225:PRO:HD2	1:B:227:ASN:OD1	1.96	0.65
1:B:249:VAL:H	1:B:260:ILE:CG2	2.09	0.65
1:A:301:VAL:O	1:A:301:VAL:CG2	2.44	0.65
1:B:225:PRO:O	1:B:226:GLU:HG3	1.96	0.65
1:A:77:LEU:O	1:A:77:LEU:HD12	1.97	0.65
1:B:260:ILE:HG12	1:B:297:LEU:HD22	1.78	0.64
1:B:36:SER:O	1:B:114:SER:O	2.16	0.64
1:A:231:ARG:C	1:A:234:GLU:H	2.01	0.64
1:B:249:VAL:HG12	1:B:260:ILE:HG22	1.80	0.64
1:B:283:CYS:C	1:B:285:LEU:H	1.99	0.64
1:A:301:VAL:O	1:A:302:ALA:C	2.37	0.64
1:B:244:LEU:HD11	1:B:250:ILE:CG1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ILE:O	1:B:241:ILE:HD13	1.97	0.63
1:B:260:ILE:HG23	1:B:261:PRO:HD3	1.79	0.63
1:B:65:SER:CA	2:B:333:HOH:O	2.45	0.63
1:B:225:PRO:HD2	1:B:227:ASN:CG	2.18	0.63
1:B:114:SER:C	1:B:116:SER:H	2.00	0.63
1:B:290:THR:HG22	1:B:290:THR:O	1.99	0.63
1:B:109:THR:HG23	1:B:126:ARG:HA	1.79	0.63
1:B:32:VAL:HG22	1:B:110:ILE:HG12	1.79	0.62
1:B:168:PHE:CZ	1:B:172:ARG:HD2	2.34	0.62
1:A:260:ILE:HG12	1:A:297:LEU:HD22	1.80	0.62
1:A:32:VAL:HG22	1:A:110:ILE:HG12	1.80	0.62
1:A:97:THR:O	1:A:100:ILE:HG22	1.99	0.62
1:A:225:PRO:HD2	1:A:227:ASN:OD1	1.98	0.62
1:A:225:PRO:HD2	1:A:227:ASN:CG	2.20	0.62
1:B:199:VAL:O	1:B:203:ILE:HG13	2.00	0.62
1:A:290:THR:O	1:A:290:THR:HG22	1.99	0.62
1:A:44:SER:HB3	1:B:81:ALA:O	2.00	0.61
1:A:147:VAL:HG11	1:A:282:ILE:HD12	1.82	0.61
1:A:122:TRP:CE3	1:A:124:PRO:HG3	2.35	0.61
1:B:285:LEU:C	1:B:285:LEU:HD12	2.21	0.61
1:B:227:ASN:HA	2:B:406:HOH:O	2.00	0.60
1:A:168:PHE:CZ	1:A:172:ARG:HD2	2.36	0.60
1:B:122:TRP:CE3	1:B:124:PRO:HG3	2.35	0.60
1:B:147:VAL:HG11	1:B:282:ILE:HD12	1.82	0.60
1:A:36:SER:O	1:A:114:SER:O	2.20	0.60
1:B:130:MSE:CE	1:B:157:ARG:HG2	2.31	0.60
1:B:212:SER:H	1:B:215:ASP:HB2	1.66	0.60
1:A:137:ILE:H	1:A:137:ILE:HD12	1.65	0.59
1:A:199:VAL:O	1:A:203:ILE:HG13	2.02	0.59
1:A:213:LEU:O	1:A:217:ARG:HG3	2.01	0.59
1:A:259:ARG:HH11	1:A:259:ARG:CB	2.10	0.59
1:A:149:HIS:HD2	1:A:278:TRP:HE1	1.48	0.59
1:A:212:SER:H	1:A:215:ASP:HB2	1.67	0.59
1:A:130:MSE:CE	1:A:157:ARG:HG2	2.33	0.58
1:B:289:TYR:C	1:B:291:VAL:H	2.06	0.58
1:B:114:SER:O	1:B:115:LYS:CB	2.50	0.58
1:A:138:ILE:O	1:A:142:ILE:HG12	2.03	0.58
1:B:149:HIS:HD2	1:B:278:TRP:HE1	1.50	0.58
1:B:259:ARG:HH11	1:B:259:ARG:CB	2.12	0.58
1:A:260:ILE:CG2	1:A:261:PRO:CD	2.73	0.58
1:A:290:THR:C	1:A:292:LYS:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ILE:HG22	1:A:236:GLY:HA2	1.85	0.57
1:B:260:ILE:CG2	1:B:261:PRO:CD	2.72	0.57
1:B:260:ILE:HG13	1:B:261:PRO:N	2.20	0.57
1:A:289:TYR:C	1:A:291:VAL:H	2.07	0.56
1:B:30:ILE:HG22	1:B:75:SER:HB3	1.86	0.56
1:B:138:ILE:O	1:B:142:ILE:HG12	2.04	0.56
1:B:255:GLU:HA	2:B:400:HOH:O	2.05	0.56
1:B:291:VAL:HA	2:B:331:HOH:O	2.06	0.56
1:B:137:ILE:H	1:B:137:ILE:HD12	1.69	0.56
1:A:285:LEU:C	1:A:285:LEU:HD12	2.27	0.56
1:B:203:ILE:HG22	1:B:236:GLY:HA2	1.87	0.55
1:B:77:LEU:O	1:B:77:LEU:HD12	2.06	0.55
1:B:137:ILE:HG22	1:B:170:TYR:CE2	2.41	0.55
1:B:213:LEU:O	1:B:217:ARG:HG3	2.07	0.55
1:B:106:ARG:HG3	1:B:106:ARG:HH11	1.70	0.54
1:B:291:VAL:CA	2:B:331:HOH:O	2.55	0.54
1:B:290:THR:C	1:B:292:LYS:N	2.61	0.54
1:B:35:ILE:CD1	1:B:113:VAL:HB	2.38	0.54
1:A:35:ILE:CD1	1:A:113:VAL:HB	2.38	0.54
1:A:60:ILE:HD12	1:A:149:HIS:CE1	2.44	0.53
1:B:290:THR:C	1:B:292:LYS:H	2.09	0.53
1:A:44:SER:HB2	1:B:85:TYR:HB2	1.89	0.53
1:A:233:LEU:C	1:A:235:LEU:N	2.62	0.53
1:A:280:GLY:HA3	1:A:296:LYS:HA	1.91	0.53
1:B:130:MSE:SE	1:B:157:ARG:HG2	2.59	0.53
1:B:237:VAL:O	1:B:238:LYS:C	2.47	0.52
1:A:106:ARG:HH11	1:A:106:ARG:HG3	1.73	0.52
1:A:290:THR:C	1:A:292:LYS:N	2.61	0.52
1:B:301:VAL:C	1:B:302:ALA:O	2.44	0.52
1:A:249:VAL:H	1:A:260:ILE:HG22	1.75	0.52
1:B:260:ILE:HG12	1:B:297:LEU:CD2	2.39	0.52
1:B:241:ILE:CG1	1:B:249:VAL:HG21	2.40	0.52
1:B:280:GLY:HA3	1:B:296:LYS:HA	1.92	0.52
1:A:237:VAL:O	1:A:238:LYS:C	2.47	0.52
1:A:184:TYR:HB2	1:A:199:VAL:HG21	1.92	0.52
1:A:213:LEU:HB2	2:A:342:HOH:O	2.10	0.51
1:B:146:LYS:N	2:B:368:HOH:O	2.41	0.51
1:A:204:SER:O	1:A:237:VAL:HG22	2.10	0.51
1:B:60:ILE:HD12	1:B:149:HIS:CE1	2.46	0.51
1:B:113:VAL:HG12	1:B:114:SER:N	2.25	0.51
1:A:241:ILE:CG1	1:A:249:VAL:HG21	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLU:C	1:B:236:GLY:H	2.14	0.51
1:B:64:LEU:HB2	1:B:71:VAL:HG21	1.92	0.51
1:A:130:MSE:SE	1:A:157:ARG:HG2	2.61	0.51
1:B:225:PRO:HD2	1:B:227:ASN:HD21	1.76	0.51
1:A:119:THR:C	1:A:120:PRO:O	2.49	0.51
1:A:260:ILE:HG13	1:A:261:PRO:N	2.25	0.51
1:B:229:VAL:HG12	1:B:229:VAL:O	2.10	0.50
1:A:27:LEU:C	1:A:27:LEU:HD23	2.32	0.49
1:A:244:LEU:HD11	1:A:250:ILE:HG13	1.94	0.49
1:A:46:SER:HB2	1:A:49:TYR:OH	2.12	0.49
1:A:225:PRO:HD2	1:A:227:ASN:HD21	1.77	0.49
1:B:233:LEU:C	1:B:235:LEU:N	2.63	0.49
1:A:28:GLY:HA3	1:A:57:PRO:HG2	1.94	0.49
1:A:137:ILE:CD1	1:A:137:ILE:N	2.73	0.49
1:A:134:GLU:HG3	1:A:163:THR:HB	1.93	0.49
1:A:137:ILE:HG22	1:A:170:TYR:CE2	2.48	0.49
1:A:229:VAL:HG12	1:A:229:VAL:O	2.12	0.49
1:B:28:GLY:HA3	1:B:57:PRO:HG2	1.94	0.49
1:A:30:ILE:HG22	1:A:75:SER:HB3	1.95	0.49
1:B:150:LEU:HD22	1:B:151:SER:N	2.28	0.49
1:B:297:LEU:HD23	2:B:380:HOH:O	2.13	0.48
1:A:64:LEU:HB2	1:A:71:VAL:HG21	1.95	0.48
1:B:22:LEU:N	2:B:355:HOH:O	2.46	0.48
1:A:234:GLU:C	1:A:236:GLY:H	2.17	0.48
1:B:46:SER:HB2	1:B:49:TYR:OH	2.13	0.48
1:A:101:GLN:NE2	1:A:132:LEU:HD12	2.28	0.48
1:B:137:ILE:N	1:B:137:ILE:CD1	2.77	0.48
1:A:35:ILE:HD12	1:A:113:VAL:HB	1.96	0.48
1:B:143:LYS:O	1:B:146:LYS:HA	2.13	0.48
1:B:184:TYR:HB2	1:B:199:VAL:HG21	1.95	0.48
1:B:157:ARG:HD2	1:B:158:LYS:HE2	1.96	0.48
1:A:76:ARG:HG2	1:A:128:ALA:HB1	1.96	0.48
1:B:210:LYS:NZ	1:B:210:LYS:HB3	2.28	0.47
1:A:283:CYS:C	1:A:285:LEU:N	2.67	0.47
1:B:76:ARG:HG2	1:B:128:ALA:HB1	1.97	0.47
1:B:134:GLU:HG3	1:B:163:THR:HB	1.96	0.47
1:A:80:ASP:OD1	1:A:107:ARG:HD3	2.15	0.47
1:B:155:LEU:O	1:B:161:ARG:HB2	2.14	0.47
1:B:256:GLU:OE2	1:B:258:ILE:HD11	2.14	0.47
1:B:106:ARG:NH1	1:B:106:ARG:HG3	2.28	0.47
1:A:112:TYR:CE2	1:B:34:MSE:HE3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LYS:O	1:A:210:LYS:HD2	2.15	0.47
1:B:150:LEU:HD22	1:B:151:SER:H	1.78	0.47
1:A:283:CYS:O	1:A:285:LEU:N	2.48	0.47
1:A:76:ARG:HH21	1:A:133:GLN:HG2	1.80	0.46
1:A:155:LEU:O	1:A:161:ARG:HB2	2.14	0.46
1:A:260:ILE:HG12	1:A:297:LEU:CD2	2.43	0.46
1:B:247:GLU:HG2	1:B:259:ARG:NH2	2.29	0.46
1:A:106:ARG:HG3	1:A:106:ARG:NH1	2.30	0.46
1:A:47:ARG:O	1:B:50:THR:HA	2.16	0.46
1:B:258:ILE:HD12	1:B:258:ILE:N	2.31	0.46
1:B:283:CYS:C	1:B:285:LEU:N	2.67	0.46
1:B:249:VAL:H	1:B:260:ILE:HG22	1.81	0.46
1:A:249:VAL:O	1:A:260:ILE:HG22	2.16	0.46
1:A:123:LEU:HD22	1:B:107:ARG:HD2	1.97	0.46
1:A:112:TYR:O	1:A:122:TRP:HA	2.16	0.46
1:A:206:ALA:O	1:A:237:VAL:HG23	2.16	0.46
1:B:217:ARG:HH11	1:B:217:ARG:HG2	1.80	0.46
1:A:149:HIS:CD2	1:A:278:TRP:NE1	2.82	0.46
1:A:210:LYS:NZ	1:A:210:LYS:HB3	2.31	0.46
1:A:250:ILE:HA	1:A:258:ILE:O	2.16	0.46
1:A:30:ILE:O	1:A:30:ILE:HG23	2.16	0.46
1:B:250:ILE:HA	1:B:258:ILE:O	2.15	0.46
1:A:140:GLU:OE2	1:A:140:GLU:N	2.49	0.45
1:A:154:ILE:HD11	1:A:160:ALA:HB1	1.98	0.45
1:A:150:LEU:HD22	1:A:151:SER:N	2.31	0.45
1:A:243:THR:HA	1:A:249:VAL:HG23	1.98	0.45
1:B:143:LYS:CB	2:B:375:HOH:O	2.64	0.45
1:B:233:LEU:O	1:B:235:LEU:N	2.49	0.45
1:B:204:SER:O	1:B:237:VAL:HG22	2.16	0.45
1:B:149:HIS:CD2	1:B:278:TRP:NE1	2.83	0.45
1:B:249:VAL:O	1:B:260:ILE:HG22	2.16	0.45
1:B:288:GLY:O	1:B:289:TYR:O	2.34	0.45
1:A:160:ALA:O	1:A:163:THR:HG23	2.17	0.45
1:A:258:ILE:HD12	1:A:258:ILE:N	2.32	0.45
1:A:247:GLU:HG2	1:A:259:ARG:NH2	2.32	0.45
1:B:140:GLU:N	1:B:140:GLU:OE2	2.50	0.45
1:A:288:GLY:O	1:A:289:TYR:O	2.35	0.45
1:B:130:MSE:HE1	1:B:157:ARG:NH1	2.32	0.45
1:A:289:TYR:C	1:A:291:VAL:N	2.70	0.45
1:B:289:TYR:C	1:B:291:VAL:N	2.70	0.45
1:A:157:ARG:HD2	1:A:158:LYS:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ASP:OD2	1:A:288:GLY:N	2.50	0.44
1:B:101:GLN:NE2	1:B:132:LEU:HD12	2.32	0.44
1:A:209:VAL:CG2	1:A:240:VAL:HB	2.47	0.44
1:B:235:LEU:O	1:B:237:VAL:HG22	2.18	0.44
1:B:30:ILE:CG2	1:B:75:SER:HB3	2.46	0.44
1:B:283:CYS:O	1:B:285:LEU:N	2.49	0.44
1:A:241:ILE:HG12	1:A:249:VAL:CG2	2.43	0.44
1:B:158:LYS:H	1:B:158:LYS:HG3	1.61	0.44
1:A:233:LEU:O	1:A:235:LEU:N	2.48	0.44
1:A:60:ILE:HD13	1:A:278:TRP:HD1	1.82	0.44
1:A:256:GLU:OE2	1:A:258:ILE:HD11	2.17	0.44
1:B:100:ILE:HG12	2:B:342:HOH:O	2.16	0.44
1:A:157:ARG:HG3	1:A:158:LYS:HE2	1.99	0.44
1:A:143:LYS:O	1:A:146:LYS:HA	2.17	0.43
1:A:130:MSE:HE1	1:A:157:ARG:NH1	2.33	0.43
1:B:22:LEU:N	2:B:374:HOH:O	2.50	0.43
1:A:209:VAL:HG23	1:A:240:VAL:HG23	2.00	0.43
1:A:36:SER:HB2	1:A:49:TYR:CE1	2.53	0.43
1:A:77:LEU:C	1:A:77:LEU:HD12	2.39	0.43
1:B:209:VAL:CG2	1:B:240:VAL:HB	2.48	0.43
1:A:217:ARG:HG2	1:A:217:ARG:HH11	1.83	0.43
1:B:206:ALA:O	1:B:237:VAL:HG23	2.19	0.43
1:A:36:SER:HB2	1:A:49:TYR:CD1	2.54	0.43
1:B:143:LYS:O	1:B:146:LYS:CB	2.66	0.43
1:B:259:ARG:HD2	2:B:369:HOH:O	2.19	0.43
1:B:244:LEU:HD11	1:B:250:ILE:HG13	1.98	0.43
1:A:217:ARG:CZ	2:A:372:HOH:O	2.67	0.43
1:B:241:ILE:HG12	1:B:249:VAL:CG2	2.46	0.43
1:B:35:ILE:HD12	1:B:113:VAL:HB	2.00	0.42
1:A:107:ARG:NH1	1:B:124:PRO:O	2.52	0.42
1:A:186:LYS:N	2:A:331:HOH:O	2.53	0.42
1:B:114:SER:C	1:B:116:SER:N	2.68	0.42
1:B:30:ILE:HG23	1:B:30:ILE:O	2.19	0.42
1:B:80:ASP:OD1	1:B:107:ARG:HD3	2.19	0.42
1:B:36:SER:HB2	1:B:49:TYR:CE1	2.54	0.42
1:B:27:LEU:HD23	1:B:27:LEU:C	2.40	0.42
1:B:71:VAL:HG12	1:B:72:ALA:N	2.35	0.42
1:B:56:SER:O	1:B:60:ILE:HG13	2.18	0.42
1:B:64:LEU:CB	1:B:71:VAL:HG21	2.49	0.42
1:B:160:ALA:O	1:B:163:THR:HG23	2.20	0.42
1:B:204:SER:HA	1:B:235:LEU:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ARG:HH21	1:B:133:GLN:HG2	1.83	0.42
1:A:178:VAL:CG2	1:A:206:ALA:HA	2.49	0.42
1:B:210:LYS:O	1:B:210:LYS:HD2	2.19	0.42
1:B:217:ARG:NH1	1:B:217:ARG:HG2	2.35	0.41
1:B:133:GLN:NE2	2:B:399:HOH:O	2.49	0.41
1:A:150:LEU:HD22	1:A:151:SER:H	1.84	0.41
1:B:30:ILE:HD12	1:B:58:ALA:CB	2.50	0.41
1:A:158:LYS:HG3	1:A:158:LYS:H	1.56	0.41
1:B:154:ILE:HD11	1:B:160:ALA:HB1	2.02	0.41
1:B:277:PHE:O	1:B:296:LYS:CB	2.69	0.41
1:A:143:LYS:O	1:A:146:LYS:CB	2.68	0.41
1:A:30:ILE:CG2	1:A:75:SER:HB3	2.51	0.41
1:B:247:GLU:HG2	1:B:259:ARG:HH22	1.86	0.41
1:A:235:LEU:O	1:A:237:VAL:HG22	2.20	0.41
1:A:244:LEU:HD11	1:A:250:ILE:HD11	2.02	0.41
1:A:64:LEU:CB	1:A:71:VAL:HG21	2.51	0.41
1:B:51:ARG:C	1:B:51:ARG:HD2	2.40	0.41
1:B:209:VAL:HG23	1:B:240:VAL:HG23	2.03	0.41
1:B:165:ILE:HA	1:B:168:PHE:HB3	2.03	0.41
1:A:210:LYS:HB3	1:A:210:LYS:HZ3	1.84	0.41
1:A:304:PHE:O	1:A:305:LYS:C	2.58	0.41
1:A:301:VAL:O	1:A:302:ALA:O	2.38	0.40
1:B:178:VAL:CG2	1:B:206:ALA:HA	2.51	0.40
1:B:189:TRP:HA	1:B:190:PRO:HD3	1.88	0.40
1:A:113:VAL:HG12	1:A:114:SER:N	2.36	0.40
1:A:225:PRO:C	1:A:226:GLU:HG3	2.40	0.40
1:A:272:GLY:N	2:A:333:HOH:O	2.54	0.40
1:B:243:THR:HA	1:B:249:VAL:HG23	2.01	0.40
1:B:257:ILE:C	1:B:258:ILE:HD12	2.42	0.40
1:A:100:ILE:HD13	1:A:100:ILE:C	2.42	0.40
1:B:137:ILE:CG2	1:B:170:TYR:CD2	2.97	0.40
1:B:198:VAL:O	1:B:202:ILE:HG13	2.22	0.40
1:B:210:LYS:HA	1:B:241:ILE:HD13	2.03	0.40
1:B:35:ILE:HD13	1:B:113:VAL:HB	2.03	0.40
1:B:157:ARG:HG3	1:B:158:LYS:HE2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	272/327 (83%)	228 (84%)	24 (9%)	20 (7%)	1	2
1	B	272/327 (83%)	232 (85%)	23 (8%)	17 (6%)	1	3
All	All	544/654 (83%)	460 (85%)	47 (9%)	37 (7%)	1	3

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	THR
1	A	120	PRO
1	A	121	ASP
1	A	223	ASP
1	A	224	SER
1	A	236	GLY
1	A	303	ALA
1	A	304	PHE
1	B	116	SER
1	B	117	THR
1	B	223	ASP
1	B	224	SER
1	B	236	GLY
1	B	260	ILE
1	A	237	VAL
1	A	260	ILE
1	A	289	TYR
1	A	305	LYS
1	B	237	VAL
1	B	289	TYR
1	A	115	LYS
1	B	302	ALA
1	A	127	GLU
1	A	234	GLU
1	B	127	GLU

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Mol	Chain	Res	Type
1	B	234	GLU
1	A	226	GLU
1	B	121	ASP
1	B	226	GLU
1	A	158	LYS
1	B	158	LYS
1	B	159	PRO
1	A	159	PRO
1	B	225	PRO
1	B	229	VAL
1	A	225	PRO
1	A	229	VAL

### 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	185/272 (68%)	165 (89%)	20 (11%)	6	19
1	B	185/272 (68%)	163 (88%)	22 (12%)	5	16
All	All	370/544 (68%)	328 (89%)	42 (11%)	5	18

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

Mol	Chain	Res	Type
1	A	77	LEU
1	A	89	VAL
1	A	100	ILE
1	A	114	SER
1	A	123	LEU
1	A	127	GLU
1	A	129	ASP
1	A	137	ILE
1	A	150	LEU
1	A	157	ARG
1	A	161	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	163	THR
1	A	165	ILE
1	A	188	LEU
1	A	210	LYS
1	A	227	ASN
1	A	237	VAL
1	A	240	VAL
1	A	241	ILE
1	A	295	ILE
1	B	77	LEU
1	B	89	VAL
1	B	100	ILE
1	B	107	ARG
1	B	114	SER
1	B	123	LEU
1	B	127	GLU
1	B	129	ASP
1	B	150	LEU
1	B	157	ARG
1	B	161	ARG
1	B	163	THR
1	B	165	ILE
1	B	188	LEU
1	B	210	LYS
1	B	227	ASN
1	B	237	VAL
1	B	240	VAL
1	B	241	ILE
1	B	295	ILE
1	B	299	ASN
1	B	301	VAL

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

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	52	HIS
1	A	84	ASN
1	A	149	HIS
1	B	52	HIS
1	B	149	HIS

### 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	276/327 (84%)	0.51	13 (4%) 31 22	25, 46, 74, 110	0
1	B	276/327 (84%)	0.45	4 (1%) 75 70	25, 45, 70, 88	0
All	All	552/654 (84%)	0.48	17 (3%) 49 39	25, 46, 73, 110	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	VAL	3.7
1	A	119	THR	3.6
1	A	225	PRO	3.5
1	B	260	ILE	3.5
1	A	117	THR	3.3
1	A	120	PRO	3.2
1	A	223	ASP	3.0
1	B	223	ASP	2.6
1	A	213	LEU	2.4
1	A	42	SER	2.4
1	A	260	ILE	2.4
1	B	291	VAL	2.3
1	A	258	ILE	2.3
1	B	259	ARG	2.2
1	A	259	ARG	2.2
1	A	244	LEU	2.2
1	A	141	LEU	2.1

### 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.