



# Full wwPDB X-ray Structure Validation Report i

Jun 16, 2024 – 11:29 PM EDT

PDB ID : 5LL2  
Title : Structure of Isoleucine 2-epimerase from Lactobacillus buchneri (apo form)  
Authors : Reiser, J.-B.; Awad, R.; Gans, P.  
Deposited on : 2016-07-26  
Resolution : 2.60 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 i 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

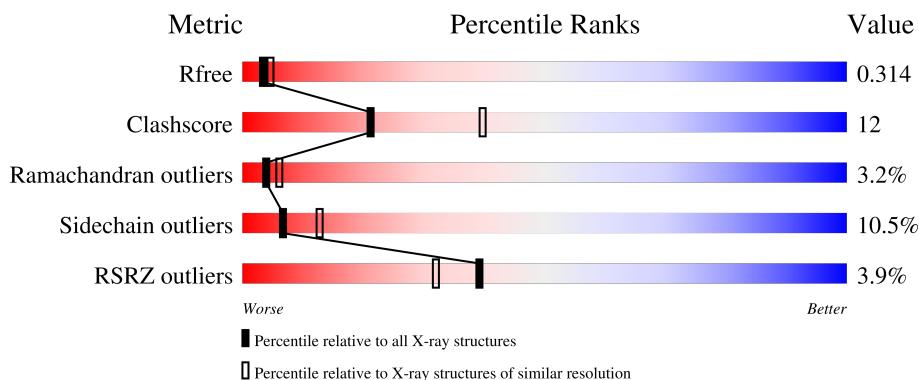
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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.



## 2 Entry composition [\(i\)](#)

There are 2 unique types of molecules in this entry. The entry contains 12578 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 Isoleucine 2-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	A	409	Total	C 3151	N 2007	O 526	S 602	16	0	1	0
1	B	409	Total	C 3146	N 2005	O 526	S 599	16	0	0	0
1	C	407	Total	C 3134	N 1997	O 524	S 597	16	0	0	0
1	D	405	Total	C 3121	N 1990	O 522	S 593	16	0	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	MET	-	initiating methionine	UNP M1GRN3
A	-28	GLY	-	expression tag	UNP M1GRN3
A	-27	SER	-	expression tag	UNP M1GRN3
A	-26	SER	-	expression tag	UNP M1GRN3
A	-25	HIS	-	expression tag	UNP M1GRN3
A	-24	HIS	-	expression tag	UNP M1GRN3
A	-23	HIS	-	expression tag	UNP M1GRN3
A	-22	HIS	-	expression tag	UNP M1GRN3
A	-21	HIS	-	expression tag	UNP M1GRN3
A	-20	HIS	-	expression tag	UNP M1GRN3
A	-19	SER	-	expression tag	UNP M1GRN3
A	-18	SER	-	expression tag	UNP M1GRN3
A	-17	GLY	-	expression tag	UNP M1GRN3
A	-16	GLU	-	expression tag	UNP M1GRN3
A	-15	ASN	-	expression tag	UNP M1GRN3
A	-14	LEU	-	expression tag	UNP M1GRN3
A	-13	TYR	-	expression tag	UNP M1GRN3
A	-12	PHE	-	expression tag	UNP M1GRN3
A	-11	GLN	-	expression tag	UNP M1GRN3
A	-10	GLY	-	expression tag	UNP M1GRN3
A	-9	HIS	-	expression tag	UNP M1GRN3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP M1GRN3
A	-7	ALA	-	expression tag	UNP M1GRN3
A	-6	SER	-	expression tag	UNP M1GRN3
A	-5	GLY	-	expression tag	UNP M1GRN3
A	-4	SER	-	expression tag	UNP M1GRN3
A	-3	GLU	-	expression tag	UNP M1GRN3
A	-2	PHE	-	expression tag	UNP M1GRN3
A	-1	GLU	-	expression tag	UNP M1GRN3
A	0	LEU	-	expression tag	UNP M1GRN3
B	-29	MET	-	initiating methionine	UNP M1GRN3
B	-28	GLY	-	expression tag	UNP M1GRN3
B	-27	SER	-	expression tag	UNP M1GRN3
B	-26	SER	-	expression tag	UNP M1GRN3
B	-25	HIS	-	expression tag	UNP M1GRN3
B	-24	HIS	-	expression tag	UNP M1GRN3
B	-23	HIS	-	expression tag	UNP M1GRN3
B	-22	HIS	-	expression tag	UNP M1GRN3
B	-21	HIS	-	expression tag	UNP M1GRN3
B	-20	HIS	-	expression tag	UNP M1GRN3
B	-19	SER	-	expression tag	UNP M1GRN3
B	-18	SER	-	expression tag	UNP M1GRN3
B	-17	GLY	-	expression tag	UNP M1GRN3
B	-16	GLU	-	expression tag	UNP M1GRN3
B	-15	ASN	-	expression tag	UNP M1GRN3
B	-14	LEU	-	expression tag	UNP M1GRN3
B	-13	TYR	-	expression tag	UNP M1GRN3
B	-12	PHE	-	expression tag	UNP M1GRN3
B	-11	GLN	-	expression tag	UNP M1GRN3
B	-10	GLY	-	expression tag	UNP M1GRN3
B	-9	HIS	-	expression tag	UNP M1GRN3
B	-8	MET	-	expression tag	UNP M1GRN3
B	-7	ALA	-	expression tag	UNP M1GRN3
B	-6	SER	-	expression tag	UNP M1GRN3
B	-5	GLY	-	expression tag	UNP M1GRN3
B	-4	SER	-	expression tag	UNP M1GRN3
B	-3	GLU	-	expression tag	UNP M1GRN3
B	-2	PHE	-	expression tag	UNP M1GRN3
B	-1	GLU	-	expression tag	UNP M1GRN3
B	0	LEU	-	expression tag	UNP M1GRN3
C	-29	MET	-	initiating methionine	UNP M1GRN3
C	-28	GLY	-	expression tag	UNP M1GRN3
C	-27	SER	-	expression tag	UNP M1GRN3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-26	SER	-	expression tag	UNP M1GRN3
C	-25	HIS	-	expression tag	UNP M1GRN3
C	-24	HIS	-	expression tag	UNP M1GRN3
C	-23	HIS	-	expression tag	UNP M1GRN3
C	-22	HIS	-	expression tag	UNP M1GRN3
C	-21	HIS	-	expression tag	UNP M1GRN3
C	-20	HIS	-	expression tag	UNP M1GRN3
C	-19	SER	-	expression tag	UNP M1GRN3
C	-18	SER	-	expression tag	UNP M1GRN3
C	-17	GLY	-	expression tag	UNP M1GRN3
C	-16	GLU	-	expression tag	UNP M1GRN3
C	-15	ASN	-	expression tag	UNP M1GRN3
C	-14	LEU	-	expression tag	UNP M1GRN3
C	-13	TYR	-	expression tag	UNP M1GRN3
C	-12	PHE	-	expression tag	UNP M1GRN3
C	-11	GLN	-	expression tag	UNP M1GRN3
C	-10	GLY	-	expression tag	UNP M1GRN3
C	-9	HIS	-	expression tag	UNP M1GRN3
C	-8	MET	-	expression tag	UNP M1GRN3
C	-7	ALA	-	expression tag	UNP M1GRN3
C	-6	SER	-	expression tag	UNP M1GRN3
C	-5	GLY	-	expression tag	UNP M1GRN3
C	-4	SER	-	expression tag	UNP M1GRN3
C	-3	GLU	-	expression tag	UNP M1GRN3
C	-2	PHE	-	expression tag	UNP M1GRN3
C	-1	GLU	-	expression tag	UNP M1GRN3
C	0	LEU	-	expression tag	UNP M1GRN3
D	-29	MET	-	initiating methionine	UNP M1GRN3
D	-28	GLY	-	expression tag	UNP M1GRN3
D	-27	SER	-	expression tag	UNP M1GRN3
D	-26	SER	-	expression tag	UNP M1GRN3
D	-25	HIS	-	expression tag	UNP M1GRN3
D	-24	HIS	-	expression tag	UNP M1GRN3
D	-23	HIS	-	expression tag	UNP M1GRN3
D	-22	HIS	-	expression tag	UNP M1GRN3
D	-21	HIS	-	expression tag	UNP M1GRN3
D	-20	HIS	-	expression tag	UNP M1GRN3
D	-19	SER	-	expression tag	UNP M1GRN3
D	-18	SER	-	expression tag	UNP M1GRN3
D	-17	GLY	-	expression tag	UNP M1GRN3
D	-16	GLU	-	expression tag	UNP M1GRN3
D	-15	ASN	-	expression tag	UNP M1GRN3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	LEU	-	expression tag	UNP M1GRN3
D	-13	TYR	-	expression tag	UNP M1GRN3
D	-12	PHE	-	expression tag	UNP M1GRN3
D	-11	GLN	-	expression tag	UNP M1GRN3
D	-10	GLY	-	expression tag	UNP M1GRN3
D	-9	HIS	-	expression tag	UNP M1GRN3
D	-8	MET	-	expression tag	UNP M1GRN3
D	-7	ALA	-	expression tag	UNP M1GRN3
D	-6	SER	-	expression tag	UNP M1GRN3
D	-5	GLY	-	expression tag	UNP M1GRN3
D	-4	SER	-	expression tag	UNP M1GRN3
D	-3	GLU	-	expression tag	UNP M1GRN3
D	-2	PHE	-	expression tag	UNP M1GRN3
D	-1	GLU	-	expression tag	UNP M1GRN3
D	0	LEU	-	expression tag	UNP M1GRN3

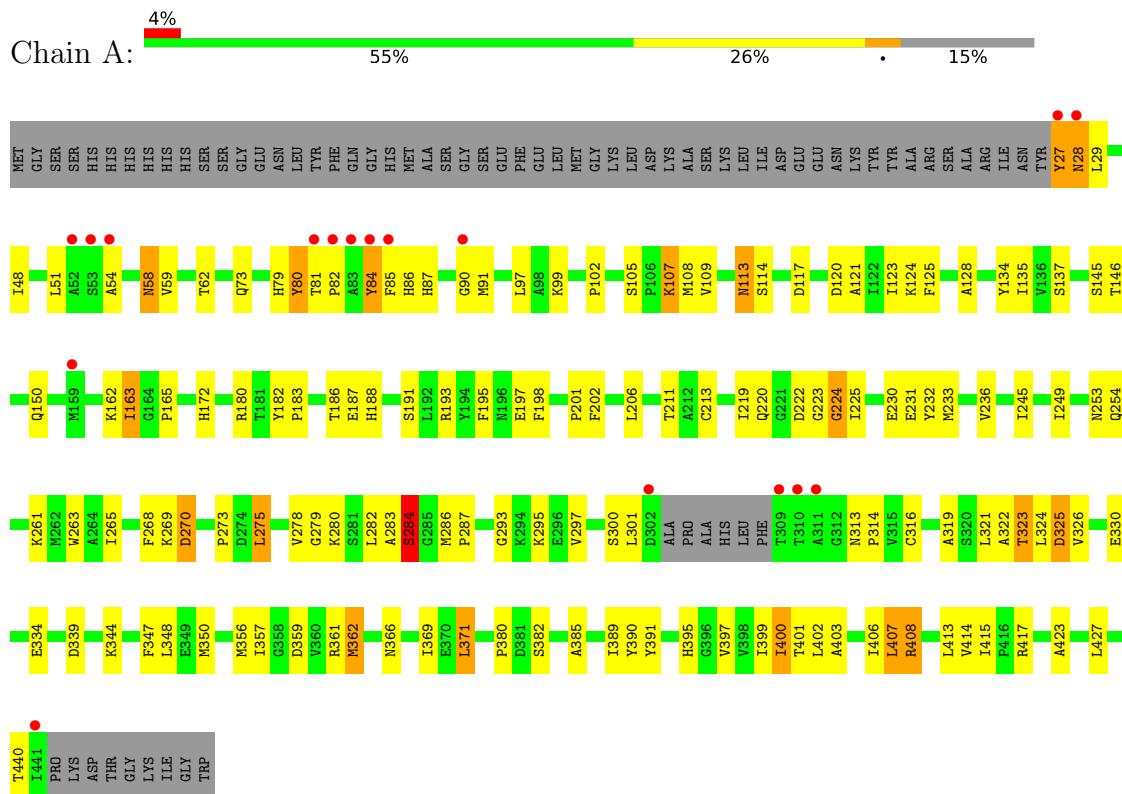
- Molecule 2 is water.

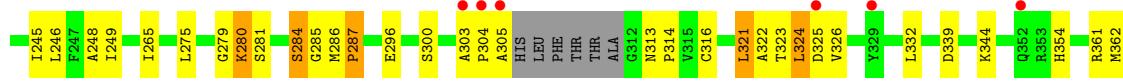
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	10	Total O 10 10	0	0
2	B	3	Total O 3 3	0	0
2	C	8	Total O 8 8	0	0
2	D	5	Total O 5 5	0	0

### 3 Residue-property plots

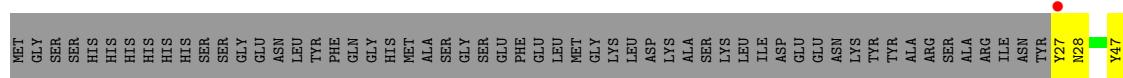
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Isoleucine 2-epimerase

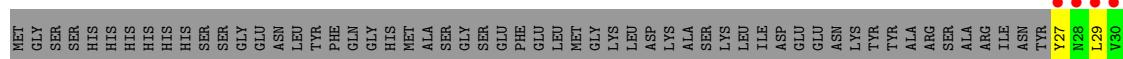




- Molecule 1: Isoleucine 2-epimerase



- Molecule 1: Isoleucine 2-epimerase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.16 Å   161.78 Å   186.17 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	19.93 – 2.60 19.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.93-2.60) 98.9 (19.93-2.60)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	33.57 (at 2.59 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
$R$ , $R_{free}$	0.244 , 0.316 0.243 , 0.314	Depositor DCC
$R_{free}$ test set	2752 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 39.3	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.39$ , $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	12578	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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  $< |L| >$ ,  $< L^2 >$  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	0.66	0/3225	0.88	3/4374 (0.1%)
1	B	0.65	0/3218	0.90	1/4365 (0.0%)
1	C	0.65	0/3205	0.85	3/4346 (0.1%)
1	D	0.66	0/3192	0.89	5/4328 (0.1%)
All	All	0.65	0/12840	0.88	12/17413 (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	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	D	275	LEU	CA-CB-CG	7.07	131.56	115.30
1	D	420	LEU	CA-CB-CG	6.58	130.43	115.30
1	D	39	LEU	CA-CB-CG	6.00	129.09	115.30
1	C	222	ASP	CB-CG-OD1	5.95	123.65	118.30
1	D	29	LEU	CA-CB-CG	5.89	128.85	115.30
1	D	250	ASP	CB-CG-OD1	5.75	123.48	118.30
1	B	51	LEU	CA-CB-CG	5.55	128.06	115.30
1	C	222	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	407	LEU	CA-CB-CG	5.26	127.39	115.30
1	C	407	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	427	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	324	LEU	CB-CG-CD1	5.07	119.62	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	GLY	Peptide
1	D	159	MET	Peptide

## 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	3151	0	3114	96	0
1	B	3146	0	3107	78	0
1	C	3134	0	3095	100	0
1	D	3121	0	3086	55	0
2	A	10	0	0	4	0
2	B	3	0	0	0	0
2	C	8	0	0	1	0
2	D	5	0	0	0	0
All	All	12578	0	12402	302	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 12.

All (302) 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:C:52:ALA:CB	1:C:408:ARG:HD2	1.69	1.23
1:A:81:THR:HB	1:A:84:TYR:OH	1.49	1.12
1:C:52:ALA:HB2	1:C:408:ARG:HD2	1.28	1.10
1:A:81:THR:HB	1:A:84:TYR:CZ	2.01	0.95
1:C:52:ALA:HB1	1:C:408:ARG:HD2	1.51	0.91
1:C:54:ALA:HB1	1:C:280:LYS:NZ	1.84	0.91
1:C:52:ALA:HB2	1:C:408:ARG:CD	2.01	0.89
1:D:319:ALA:O	1:D:323:THR:HG23	1.72	0.89
1:D:416:PRO:HD2	1:D:419:GLN:OE1	1.78	0.84
1:C:54:ALA:HB1	1:C:280:LYS:HZ3	1.43	0.83
1:A:81:THR:CB	1:A:84:TYR:OH	2.25	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:VAL:HG12	1:C:280:LYS:HE3	1.60	0.81
1:C:397:VAL:HG11	1:C:426:VAL:HG11	1.63	0.80
1:B:344:LYS:HD3	1:B:362:MET:HB3	1.66	0.77
1:C:130:THR:HB	1:C:132:ARG:HD2	1.66	0.77
1:C:285:GLY:HA3	1:D:79:HIS:HB3	1.65	0.77
1:A:81:THR:O	1:A:84:TYR:CE1	2.40	0.75
1:B:56:ALA:HA	1:B:281:SER:HA	1.69	0.74
1:B:222:ASP:HA	1:B:402:LEU:HD22	1.67	0.74
1:A:51:LEU:HD13	1:A:400:ILE:HG12	1.71	0.73
1:C:56:ALA:HA	1:C:280:LYS:HB3	1.70	0.72
1:A:389:ILE:HG22	1:A:399:ILE:HG23	1.69	0.72
1:C:124:LYS:NZ	1:D:150:GLN:HE22	1.88	0.71
1:B:50:LEU:HD12	1:B:399:ILE:HB	1.72	0.71
1:C:123:ILE:HD11	1:C:152:LEU:HD11	1.73	0.71
1:C:402:LEU:HD11	1:C:408:ARG:HE	1.54	0.71
1:B:304:PRO:O	1:B:305:ALA:C	2.30	0.70
1:D:278:VAL:HB	1:D:290:ALA:HB3	1.72	0.70
1:A:195:PHE:O	1:A:198:PHE:HB3	1.92	0.69
1:C:397:VAL:CG1	1:C:426:VAL:HG11	2.21	0.69
1:A:81:THR:HB	1:A:84:TYR:CE1	2.28	0.68
1:A:283:ALA:CB	2:A:507:HOH:O	2.42	0.67
1:C:52:ALA:CB	1:C:408:ARG:CD	2.60	0.67
1:A:249:ILE:HG21	1:A:265:ILE:HD13	1.78	0.66
1:B:422:GLN:O	1:B:426:VAL:HG23	1.96	0.66
1:C:55:SER:HB2	1:C:253:ASN:HA	1.76	0.65
1:B:249:ILE:HD13	1:B:265:ILE:HB	1.78	0.65
1:B:322:ALA:O	1:B:326:VAL:HG23	1.96	0.65
1:A:124:LYS:HE2	1:B:150:GLN:HE22	1.62	0.64
1:C:52:ALA:HB3	1:C:400:ILE:HD11	1.79	0.64
1:C:418:GLU:O	1:C:422:GLN:HB2	1.97	0.64
1:B:202:PHE:HE1	1:B:211:THR:HG21	1.64	0.63
1:C:54:ALA:HB1	1:C:280:LYS:CE	2.28	0.63
1:B:234:GLN:O	1:B:238:LYS:HG3	1.99	0.63
1:C:386:THR:HA	1:C:389:ILE:HG12	1.80	0.63
1:C:327:ILE:HG12	1:C:332:LEU:HD12	1.81	0.62
1:B:51:LEU:HD13	1:B:400:ILE:HD11	1.81	0.62
1:A:81:THR:N	1:A:84:TYR:HE1	1.99	0.61
1:D:143:HIS:HD2	1:D:152:LEU:HB3	1.64	0.61
1:C:252:VAL:HG12	1:C:280:LYS:CE	2.31	0.61
1:C:51:LEU:O	1:C:52:ALA:CB	2.49	0.61
1:A:97:LEU:HD21	1:A:282:LEU:HD11	1.81	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ARG:HG2	1:C:162:LYS:HG3	1.82	0.61
1:A:326:VAL:O	1:A:330:GLU:HB2	2.01	0.60
1:B:126:ALA:HA	1:B:246:LEU:HD12	1.83	0.59
1:B:249:ILE:HG21	1:B:265:ILE:HD13	1.83	0.59
1:A:283:ALA:HB1	2:A:507:HOH:O	2.02	0.59
1:D:237:TYR:CE1	1:D:241:HIS:CE1	2.91	0.59
1:C:97:LEU:CD2	1:C:324:LEU:HD21	2.34	0.58
1:B:385:ALA:O	1:B:389:ILE:HG12	2.04	0.58
1:A:165:PRO:HG3	1:C:165:PRO:HB3	1.86	0.58
1:C:136:VAL:HB	1:C:214:VAL:HG22	1.87	0.57
1:B:126:ALA:HB1	1:B:213:CYS:HB2	1.87	0.56
1:A:369:ILE:HB	1:A:407:LEU:HB2	1.87	0.56
1:C:50:LEU:HA	1:C:411:PRO:HA	1.86	0.56
1:C:263:TRP:HB2	1:C:266:GLN:HE21	1.70	0.56
1:D:119:ASN:HD22	1:D:143:HIS:HB3	1.70	0.56
1:B:43:ASP:HB2	1:B:45:ASN:OD1	2.06	0.56
1:A:322:ALA:O	1:A:325:ASP:HB2	2.05	0.56
1:B:58:ASN:O	1:B:413:LEU:HB2	2.06	0.56
1:A:58:ASN:HB3	1:A:413:LEU:HG	1.87	0.56
1:B:137:SER:HB3	1:B:152:LEU:HD22	1.86	0.55
1:C:361:ARG:NH1	1:C:370:GLU:OE1	2.36	0.55
1:B:211:THR:O	1:B:245:ILE:HG12	2.05	0.55
1:B:120:ASP:OD1	1:B:146:THR:OG1	2.24	0.55
1:A:230:GLU:HA	1:A:268:PHE:CD2	2.42	0.55
1:C:313:ASN:HB3	1:C:316:CYS:HB2	1.88	0.55
1:A:81:THR:CG2	1:A:82:PRO:CD	2.85	0.55
1:B:202:PHE:CE1	1:B:211:THR:HG21	2.42	0.54
1:C:54:ALA:CB	1:C:280:LYS:HE2	2.37	0.54
1:A:87:HIS:CE1	1:A:90:GLY:HA3	2.43	0.54
1:A:81:THR:O	1:A:84:TYR:CD1	2.60	0.54
1:A:193:ARG:O	1:A:197:GLU:HG2	2.07	0.54
1:A:385:ALA:HB1	1:A:401:THR:HG21	1.88	0.54
1:B:150:GLN:HG2	1:B:160:THR:CG2	2.38	0.54
1:A:86:HIS:O	1:B:31:ILE:HG22	2.08	0.53
1:B:204:SER:OG	1:B:205:PHE:N	2.41	0.53
1:B:248:ALA:HA	1:B:275:LEU:O	2.08	0.53
1:C:132:ARG:O	1:C:212:ALA:HB2	2.08	0.53
1:C:193:ARG:O	1:C:197:GLU:HG2	2.09	0.53
1:B:402:LEU:HG	1:B:408:ARG:HG2	1.90	0.53
1:B:365:LEU:HD13	1:B:411:PRO:HG2	1.91	0.53
1:C:124:LYS:HZ3	1:D:150:GLN:HE22	1.57	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLN:HE21	1:A:163:ILE:HD11	1.74	0.52
1:B:171:VAL:HG21	1:B:206:LEU:HG22	1.91	0.52
1:B:354:HIS:HE1	1:B:432:THR:HG23	1.74	0.52
1:C:97:LEU:HD23	1:C:324:LEU:HD21	1.91	0.52
1:D:392:ALA:HB1	1:D:397:VAL:HG23	1.92	0.52
1:D:249:ILE:HG12	1:D:273:PRO:HB3	1.92	0.52
1:C:282:LEU:HG	1:C:288:LEU:HD23	1.90	0.52
1:A:128:ALA:HA	1:B:162:LYS:HB3	1.92	0.52
1:C:87:HIS:O	1:C:91:MET:HG3	2.09	0.52
1:A:230:GLU:HA	1:A:268:PHE:CE2	2.45	0.52
1:C:213:CYS:HA	1:C:245:ILE:CG2	2.40	0.52
1:A:81:THR:CG2	1:A:82:PRO:HD2	2.40	0.52
1:C:283:ALA:C	1:C:285:GLY:H	2.14	0.51
1:D:216:ILE:O	1:D:249:ILE:HA	2.09	0.51
1:A:123:ILE:HG23	1:A:135:ILE:HD11	1.92	0.51
1:B:49:ASP:OD1	1:B:50:LEU:N	2.43	0.51
1:A:253:ASN:OD1	1:A:254:GLN:NE2	2.42	0.51
1:C:319:ALA:O	1:C:323:THR:HG23	2.10	0.51
1:B:344:LYS:HB2	1:B:362:MET:HG2	1.92	0.51
1:C:141:SER:HB2	1:C:217:GLU:OE1	2.11	0.51
1:D:385:ALA:HB1	1:D:401:THR:HG21	1.93	0.51
1:A:344:LYS:HG3	1:A:362:MET:HB3	1.92	0.51
1:B:193:ARG:O	1:B:197:GLU:HG2	2.10	0.50
1:B:284:SER:OG	1:B:323:THR:CG2	2.60	0.50
1:D:127:ARG:HG2	1:D:132:ARG:O	2.11	0.50
1:B:286:MET:HB3	1:B:316:CYS:SG	2.52	0.50
1:B:339:ASP:HB3	1:B:365:LEU:HD21	1.94	0.50
1:C:54:ALA:HB1	1:C:280:LYS:HE2	1.93	0.50
1:C:123:ILE:HG23	1:C:135:ILE:HG13	1.92	0.50
1:A:193:ARG:HG3	1:D:182:TYR:OH	2.10	0.50
1:A:80:TYR:HE2	1:B:61:HIS:HE2	1.60	0.50
1:A:81:THR:HG22	1:A:82:PRO:HD2	1.94	0.50
1:C:363:TRP:O	1:C:366:ASN:HB3	2.12	0.50
1:B:119:ASN:OD1	1:B:215:LEU:HD11	2.12	0.49
1:A:313:ASN:HB3	1:A:316:CYS:SG	2.52	0.49
1:A:403:ALA:HB3	1:A:406:ILE:HD12	1.94	0.49
1:D:108:MET:HG3	1:D:295:LYS:HG3	1.93	0.49
1:A:124:LYS:CE	1:B:150:GLN:HE22	2.26	0.49
1:C:213:CYS:HA	1:C:245:ILE:HG22	1.94	0.49
1:A:339:ASP:OD1	1:A:417:ARG:NH2	2.45	0.49
1:B:370:GLU:HA	1:B:406:ILE:HA	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:ASP:O	1:D:50:LEU:HD23	2.12	0.49
1:C:76:LYS:HE2	1:D:33:HIS:HB3	1.95	0.49
1:A:108:MET:SD	1:A:295:LYS:HG3	2.53	0.48
1:D:129:TYR:CD2	1:D:246:LEU:HD21	2.47	0.48
1:A:220:GLN:HE21	1:A:223:GLY:HA3	1.77	0.48
1:C:102:PRO:HD3	1:C:263:TRP:CD1	2.48	0.48
1:C:54:ALA:O	1:C:56:ALA:N	2.46	0.48
1:C:275:LEU:HD23	1:C:293:GLY:HA3	1.94	0.48
1:A:85:PHE:HB3	1:B:31:ILE:HB	1.95	0.48
1:A:59:VAL:HG13	1:A:326:VAL:HG11	1.96	0.48
1:C:124:LYS:HB3	1:C:301:LEU:HD11	1.96	0.48
1:C:127:ARG:CZ	1:D:165:PRO:HD2	2.44	0.48
1:D:225:ILE:HG21	1:D:367:GLY:HA2	1.95	0.48
1:A:319:ALA:O	1:A:323:THR:HG22	2.14	0.48
1:B:161:ARG:HD3	1:C:209:ASP:OD2	2.14	0.48
1:D:362:MET:HA	1:D:366:ASN:O	2.14	0.48
1:B:397:VAL:HG11	1:B:426:VAL:HB	1.95	0.47
1:C:70:ILE:HG23	1:C:315:VAL:HG13	1.96	0.47
1:D:39:LEU:HD21	1:D:49:ASP:CG	2.35	0.47
1:A:347:PHE:HA	1:A:350:MET:HB2	1.96	0.47
1:B:138:TYR:CZ	1:B:216:ILE:HD12	2.49	0.47
1:D:278:VAL:HG11	1:D:282:LEU:HD13	1.95	0.47
1:C:233:MET:HG3	1:C:271:ILE:HD13	1.96	0.47
1:A:180:ARG:HH21	1:A:380:PRO:HD3	1.79	0.47
1:B:237:TYR:CZ	1:B:241:HIS:HE1	2.33	0.47
1:D:335:LYS:HD3	1:D:413:LEU:O	2.15	0.47
1:C:219:ILE:HG12	1:C:227:LYS:HB2	1.96	0.47
1:B:180:ARG:NH1	1:B:370:GLU:OE2	2.34	0.47
1:A:79:HIS:CB	1:B:285:GLY:HA3	2.46	0.46
1:A:222:ASP:HA	1:A:402:LEU:HD22	1.96	0.46
1:A:213:CYS:HA	1:A:245:ILE:HG22	1.98	0.46
1:A:81:THR:CA	1:A:84:TYR:HE1	2.29	0.46
1:A:322:ALA:O	1:A:326:VAL:HG23	2.16	0.46
1:C:336:SER:HB2	1:C:413:LEU:HD22	1.98	0.46
1:B:402:LEU:O	1:B:403:ALA:C	2.54	0.46
1:A:202:PHE:HE1	1:A:211:THR:HG21	1.81	0.46
1:B:237:TYR:CZ	1:B:241:HIS:CE1	3.04	0.46
1:B:313:ASN:HA	1:B:314:PRO:HD3	1.71	0.46
1:C:54:ALA:CB	1:C:280:LYS:HZ3	2.23	0.46
1:C:109:VAL:HG12	1:C:292:ILE:HG23	1.98	0.46
1:C:389:ILE:HG21	1:C:401:THR:HG23	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ILE:HG12	1:A:273:PRO:HB3	1.99	0.45
1:B:361:ARG:HB3	1:B:363:TRP:CZ3	2.52	0.45
1:A:54:ALA:O	1:A:280:LYS:HD3	2.17	0.45
1:A:105:SER:O	1:A:107:LYS:HG2	2.16	0.45
1:C:51:LEU:HD22	1:C:51:LEU:HA	1.62	0.45
1:A:81:THR:HG22	1:A:82:PRO:CD	2.46	0.45
1:B:204:SER:OG	1:B:205:PHE:HD1	1.99	0.45
1:C:278:VAL:O	1:C:289:SER:HA	2.16	0.45
1:A:219:ILE:O	1:A:254:GLN:HG3	2.17	0.45
1:C:93:LEU:HB2	1:C:321:LEU:HD13	1.98	0.45
1:C:195:PHE:CE2	1:C:199:LYS:HD2	2.51	0.45
1:A:48:ILE:HG21	1:A:423:ALA:HB2	1.99	0.45
1:A:62:THR:HG21	1:B:75:GLN:O	2.17	0.45
1:A:300:SER:O	1:A:301:LEU:HD23	2.16	0.45
1:B:207:PRO:HB3	1:C:161:ARG:HH12	1.82	0.45
1:C:327:ILE:HG23	1:C:332:LEU:HB2	1.99	0.45
1:C:402:LEU:HD11	1:C:408:ARG:NE	2.27	0.45
1:D:385:ALA:HB1	1:D:401:THR:CG2	2.47	0.45
1:D:227:LYS:HE2	1:D:268:PHE:CZ	2.52	0.45
1:D:294:LYS:HD3	1:D:296:GLU:OE1	2.17	0.45
1:C:137:SER:O	1:C:172:HIS:HA	2.16	0.45
1:B:167:LEU:HD12	1:B:168:PRO:HD2	1.99	0.44
1:A:286:MET:HE1	1:B:286:MET:CE	2.47	0.44
1:C:135:ILE:HG21	1:C:152:LEU:HD21	2.00	0.44
1:D:351:GLN:NE2	1:D:357:ILE:O	2.50	0.44
1:D:382:SER:HA	1:D:404:GLY:O	2.16	0.44
1:A:81:THR:HA	1:A:82:PRO:HD3	1.84	0.44
1:A:113:ASN:HD22	1:B:287:PRO:HB3	1.82	0.44
1:B:96:LYS:HG2	1:B:324:LEU:HD23	1.98	0.44
1:D:215:LEU:HD23	1:D:248:ALA:HB1	2.00	0.44
1:D:374:ASP:HA	1:D:375:PRO:HD2	1.62	0.44
1:A:273:PRO:HB2	1:A:275:LEU:O	2.18	0.44
1:B:48:ILE:HG21	1:B:423:ALA:HB2	1.98	0.44
1:B:88:VAL:O	1:B:91:MET:HB2	2.17	0.44
1:B:279:GLY:O	1:B:280:LYS:C	2.56	0.44
1:B:365:LEU:HD12	1:B:413:LEU:HD23	2.00	0.44
1:B:225:ILE:HG13	1:B:367:GLY:O	2.18	0.44
1:D:137:SER:O	1:D:172:HIS:HA	2.17	0.44
1:D:143:HIS:CD2	1:D:152:LEU:HB3	2.50	0.44
1:A:206:LEU:HD11	1:A:211:THR:HG22	2.00	0.44
1:A:284:SER:HB2	1:A:323:THR:HG21	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ASP:OD1	1:B:47:TYR:HE2	2.01	0.43
1:B:132:ARG:HB3	1:B:210:GLU:O	2.18	0.43
1:D:202:PHE:HE1	1:D:211:THR:HG21	1.82	0.43
1:B:127:ARG:HG2	1:B:132:ARG:O	2.18	0.43
1:A:391:TYR:CE2	1:A:395:HIS:CD2	3.07	0.43
1:B:237:TYR:CE1	1:B:241:HIS:CE1	3.05	0.43
1:B:391:TYR:CD1	1:B:430:ALA:HB2	2.54	0.43
1:C:402:LEU:HD11	1:C:408:ARG:HH21	1.84	0.43
1:D:157:LEU:HD21	1:D:403:ALA:HA	2.00	0.43
1:D:224:GLY:O	1:D:361:ARG:NH2	2.38	0.43
1:C:82:PRO:HA	1:C:85:PHE:O	2.19	0.43
1:C:402:LEU:CD1	1:C:408:ARG:HE	2.26	0.43
1:D:31:ILE:HD11	1:D:39:LEU:HB3	2.01	0.43
1:A:73:GLN:HG2	1:A:314:PRO:O	2.18	0.43
1:A:224:GLY:O	1:A:361:ARG:NH2	2.44	0.43
1:B:142:TYR:O	1:B:142:TYR:CD2	2.71	0.43
1:C:97:LEU:HD21	1:C:324:LEU:HD21	2.00	0.43
1:C:422:GLN:O	1:C:426:VAL:HG23	2.19	0.43
1:D:357:ILE:HG23	1:D:369:ILE:HG22	2.01	0.42
1:A:120:ASP:OD1	1:A:146:THR:OG1	2.34	0.42
1:A:186:THR:O	1:A:188:HIS:N	2.52	0.42
1:C:63:HIS:ND1	1:C:65:LYS:HB2	2.34	0.42
1:A:137:SER:O	1:A:172:HIS:HA	2.19	0.42
1:A:283:ALA:HB1	1:A:286:MET:HB2	2.01	0.42
1:A:87:HIS:CE1	1:A:90:GLY:CA	3.02	0.42
1:A:182:TYR:OH	1:D:193:ARG:HG3	2.19	0.42
1:C:278:VAL:O	1:C:289:SER:HB2	2.20	0.42
1:C:51:LEU:O	1:C:52:ALA:HB3	2.19	0.42
1:D:418:GLU:O	1:D:422:GLN:HG3	2.20	0.42
1:C:63:HIS:NE2	1:C:330:GLU:OE1	2.47	0.42
1:C:127:ARG:NH1	1:D:165:PRO:HD2	2.34	0.42
1:A:275:LEU:HD13	1:A:293:GLY:HA2	2.01	0.42
1:A:357:ILE:HA	1:A:371:LEU:HD12	2.00	0.42
1:B:429:ASP:O	1:B:433:ALA:N	2.48	0.42
1:C:47:TYR:HB3	1:C:398:VAL:HG23	2.02	0.42
1:C:55:SER:O	1:C:57:ILE:N	2.53	0.42
1:C:216:ILE:HG22	1:C:248:ALA:O	2.19	0.42
1:C:103:GLY:HA3	1:C:272:GLU:HG3	2.01	0.42
1:C:148:GLY:HA2	1:C:167:LEU:HD22	2.01	0.42
1:D:255:GLY:O	1:D:256:LEU:C	2.57	0.42
1:C:343:ALA:O	1:C:347:PHE:HB2	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:LYS:HB2	1:D:362:MET:HG2	2.00	0.42
1:A:27:TYR:HB2	1:B:84:TYR:O	2.20	0.41
1:A:165:PRO:HG2	1:B:168:PRO:HG2	2.02	0.41
1:A:224:GLY:HA3	1:A:406:ILE:HD13	2.02	0.41
1:A:263:TRP:HZ3	1:A:278:VAL:HG21	1.85	0.41
1:A:402:LEU:HD21	1:A:408:ARG:HH11	1.85	0.41
1:A:414:VAL:O	1:A:415:ILE:C	2.59	0.41
1:C:140:GLY:N	1:C:154:GLY:O	2.52	0.41
1:D:182:TYR:O	1:D:183:PRO:C	2.59	0.41
1:D:318:ALA:HA	1:D:321:LEU:HD22	2.02	0.41
1:A:162:LYS:HB3	1:B:128:ALA:HA	2.02	0.41
1:C:122:ILE:HD11	1:C:277:SER:HB3	2.01	0.41
1:C:249:ILE:HG12	1:C:273:PRO:HB3	2.02	0.41
1:D:358:GLY:HA3	1:D:372:VAL:HG22	2.02	0.41
1:D:374:ASP:OD2	1:D:377:THR:N	2.51	0.41
1:A:399:ILE:HG22	2:A:502:HOH:O	2.20	0.41
1:D:348:LEU:HD12	1:D:360:VAL:HG11	2.03	0.41
1:B:370:GLU:HB2	1:B:406:ILE:HG23	2.02	0.41
1:C:105:SER:HG	1:C:272:GLU:CD	2.24	0.41
1:C:400:ILE:HD13	1:D:84:TYR:CZ	2.55	0.41
1:A:102:PRO:HD3	1:A:263:TRP:CD1	2.56	0.41
1:A:286:MET:HB2	2:A:507:HOH:O	2.20	0.41
1:B:138:TYR:CE1	1:B:216:ILE:HD12	2.56	0.41
1:C:76:LYS:NZ	1:D:32:ASP:OD1	2.49	0.41
1:C:218:PRO:O	1:C:219:ILE:HG13	2.20	0.41
1:C:383:ASP:OD1	1:C:387:LYS:HE3	2.21	0.41
1:A:121:ALA:O	1:A:125:PHE:HD2	2.04	0.41
1:A:202:PHE:HA	1:A:206:LEU:O	2.20	0.41
1:A:275:LEU:HD11	1:A:297:VAL:HG11	2.03	0.41
1:C:59:VAL:HG21	1:C:323:THR:HB	2.02	0.41
1:C:253:ASN:HA	1:C:280:LYS:HZ2	1.86	0.41
1:A:134:TYR:HB2	1:A:211:THR:HA	2.03	0.40
1:A:232:TYR:O	1:A:236:VAL:HG23	2.21	0.40
1:A:287:PRO:HG2	1:B:287:PRO:HG2	2.03	0.40
1:C:351:GLN:HG3	1:C:357:ILE:HB	2.02	0.40
1:D:173:VAL:HG12	1:D:201:PRO:HG2	2.03	0.40
1:D:278:VAL:HG12	1:D:282:LEU:HD22	2.03	0.40
1:A:81:THR:CB	1:A:84:TYR:CE1	3.03	0.40
1:C:210:GLU:HG2	2:C:503:HOH:O	2.21	0.40
1:D:329:TYR:C	1:D:331:GLY:H	2.24	0.40
1:B:150:GLN:HG2	1:B:160:THR:HG21	2.02	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:GLU:OE1	1:C:251:GLU:HA	2.21	0.40
1:A:211:THR:O	1:A:245:ILE:HG23	2.22	0.40
1:C:200:LYS:HB2	1:C:201:PRO:HD2	2.03	0.40
1:D:402:LEU:O	1:D:406:ILE:HB	2.21	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	406/480 (85%)	347 (86%)	50 (12%)	9 (2%)	6 12
1	B	405/480 (84%)	339 (84%)	49 (12%)	17 (4%)	3 3
1	C	403/480 (84%)	336 (83%)	55 (14%)	12 (3%)	4 7
1	D	401/480 (84%)	326 (81%)	62 (16%)	13 (3%)	4 6
All	All	1615/1920 (84%)	1348 (84%)	216 (13%)	51 (3%)	4 6

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	GLU
1	B	62	THR
1	B	280	LYS
1	B	403	ALA
1	C	52	ALA
1	C	55	SER
1	C	56	ALA
1	D	62	THR
1	D	98	ALA
1	D	383	ASP
1	A	270	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	284	SER
1	B	58	ASN
1	B	156	SER
1	C	183	PRO
1	C	270	ASP
1	C	284	SER
1	D	375	PRO
1	A	224	GLY
1	A	366	ASN
1	A	408	ARG
1	B	158	ASN
1	B	287	PRO
1	B	366	ASN
1	D	83	ALA
1	D	188	HIS
1	D	262	MET
1	A	183	PRO
1	B	55	SER
1	B	56	ALA
1	B	321	LEU
1	B	418	GLU
1	C	54	ALA
1	D	238	LYS
1	D	280	LYS
1	A	28	ASN
1	B	438	GLU
1	C	181	THR
1	A	225	ILE
1	B	176	PRO
1	B	303	ALA
1	C	49	ASP
1	D	183	PRO
1	D	354	HIS
1	B	70	ILE
1	B	154	GLY
1	C	154	GLY
1	C	225	ILE
1	D	36	GLY
1	D	225	ILE
1	C	287	PRO

### 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	339/396 (86%)	301 (89%)	38 (11%)	6 10
1	B	337/396 (85%)	302 (90%)	35 (10%)	7 13
1	C	336/396 (85%)	303 (90%)	33 (10%)	8 15
1	D	335/396 (85%)	299 (89%)	36 (11%)	6 12
All	All	1347/1584 (85%)	1205 (90%)	142 (10%)	7 13

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	TYR
1	A	28	ASN
1	A	29	LEU
1	A	58	ASN
1	A	80	TYR
1	A	84	TYR
1	A	91	MET
1	A	99	LYS
1	A	107	LYS
1	A	109	VAL
1	A	113	ASN
1	A	114	SER
1	A	117	ASP
1	A	145	SER
1	A	163	ILE
1	A	191	SER
1	A	201	PRO
1	A	231	GLU
1	A	233	MET
1	A	261	LYS
1	A	269	LYS
1	A	270	ASP
1	A	275	LEU
1	A	284	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	321	LEU
1	A	323	THR
1	A	325	ASP
1	A	334	GLU
1	A	348	LEU
1	A	356	MET
1	A	359	ASP
1	A	362	MET
1	A	371	LEU
1	A	382	SER
1	A	390	TYR
1	A	397	VAL
1	A	400	ILE
1	A	440	THR
1	B	29	LEU
1	B	30	VAL
1	B	38	THR
1	B	42	VAL
1	B	43	ASP
1	B	46	LYS
1	B	51	LEU
1	B	53	SER
1	B	58	ASN
1	B	76	LYS
1	B	80	TYR
1	B	84	TYR
1	B	88	VAL
1	B	95	GLU
1	B	99	LYS
1	B	109	VAL
1	B	120	ASP
1	B	181	THR
1	B	211	THR
1	B	215	LEU
1	B	231	GLU
1	B	284	SER
1	B	296	GLU
1	B	300	SER
1	B	321	LEU
1	B	324	LEU
1	B	325	ASP
1	B	332	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	377	THR
1	B	406	ILE
1	B	408	ARG
1	B	427	LEU
1	B	432	THR
1	B	439	VAL
1	B	440	THR
1	C	27	TYR
1	C	28	ASN
1	C	50	LEU
1	C	51	LEU
1	C	55	SER
1	C	57	ILE
1	C	64	GLU
1	C	85	PHE
1	C	94	SER
1	C	105	SER
1	C	120	ASP
1	C	153	SER
1	C	192	LEU
1	C	209	ASP
1	C	215	LEU
1	C	222	ASP
1	C	226	ILE
1	C	231	GLU
1	C	235	LEU
1	C	269	LYS
1	C	278	VAL
1	C	302	ASP
1	C	321	LEU
1	C	338	THR
1	C	339	ASP
1	C	347	PHE
1	C	373	LYS
1	C	383	ASP
1	C	397	VAL
1	C	407	LEU
1	C	418	GLU
1	C	422	GLN
1	C	427	LEU
1	D	27	TYR
1	D	38	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	39	LEU
1	D	49	ASP
1	D	68	LYS
1	D	109	VAL
1	D	110	SER
1	D	120	ASP
1	D	157	LEU
1	D	158	ASN
1	D	169	SER
1	D	191	SER
1	D	196	ASN
1	D	213	CYS
1	D	238	LYS
1	D	241	HIS
1	D	246	LEU
1	D	250	ASP
1	D	265	ILE
1	D	269	LYS
1	D	272	GLU
1	D	275	LEU
1	D	281	SER
1	D	301	LEU
1	D	321	LEU
1	D	324	LEU
1	D	328	GLU
1	D	338	THR
1	D	383	ASP
1	D	390	TYR
1	D	400	ILE
1	D	401	THR
1	D	408	ARG
1	D	418	GLU
1	D	427	LEU
1	D	435	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	58	ASN
1	A	113	ASN
1	A	188	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	220	GLN
1	A	395	HIS
1	A	422	GLN
1	B	79	HIS
1	B	87	HIS
1	B	143	HIS
1	B	241	HIS
1	B	313	ASN
1	B	422	GLN
1	C	45	ASN
1	C	58	ASN
1	C	243	HIS
1	C	266	GLN
1	C	267	GLN
1	C	395	HIS
1	C	425	GLN
1	D	58	ASN
1	D	61	HIS
1	D	75	GLN
1	D	79	HIS
1	D	150	GLN
1	D	158	ASN
1	D	220	GLN
1	D	241	HIS
1	D	266	GLN
1	D	395	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 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 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	409/480 (85%)	0.17	17 (4%) 36 29	23, 38, 63, 92	7 (1%)
1	B	409/480 (85%)	0.13	18 (4%) 34 27	24, 40, 65, 98	7 (1%)
1	C	407/480 (84%)	0.23	16 (3%) 39 32	23, 43, 68, 134	1 (0%)
1	D	405/480 (84%)	0.09	13 (3%) 47 40	20, 40, 64, 129	1 (0%)
All	All	1630/1920 (84%)	0.16	64 (3%) 39 32	20, 41, 66, 134	16 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	PRO	7.1
1	B	156	SER	6.4
1	A	81	THR	5.9
1	B	157	LEU	5.8
1	A	83	ALA	5.7
1	A	309	THR	5.5
1	D	28	ASN	5.5
1	C	84	TYR	5.5
1	B	82	PRO	5.1
1	C	27	TYR	4.3
1	C	53	SER	4.3
1	C	82	PRO	4.1
1	D	158	ASN	3.9
1	B	304	PRO	3.8
1	B	83	ALA	3.8
1	A	84	TYR	3.8
1	B	390	TYR	3.6
1	D	80	TYR	3.4
1	D	84	TYR	3.4
1	C	81	THR	3.4
1	C	85	PHE	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	51	LEU	3.2
1	B	27	TYR	3.2
1	A	28	ASN	3.0
1	D	27	TYR	3.0
1	C	159	MET	3.0
1	A	441	ILE	2.9
1	D	83	ALA	2.9
1	C	80	TYR	2.9
1	B	84	TYR	2.9
1	D	29	LEU	2.8
1	C	55	SER	2.8
1	C	160	THR	2.8
1	D	79	HIS	2.8
1	A	311	ALA	2.8
1	A	85	PHE	2.7
1	C	83	ALA	2.6
1	B	325	ASP	2.6
1	C	439	VAL	2.6
1	B	80	TYR	2.5
1	D	301	LEU	2.5
1	A	159	MET	2.4
1	A	27	TYR	2.4
1	B	56	ALA	2.4
1	D	78	ILE	2.4
1	B	43	ASP	2.3
1	B	303	ALA	2.3
1	B	329	TYR	2.3
1	B	305	ALA	2.3
1	A	302	ASP	2.3
1	A	54	ALA	2.2
1	B	352	GLN	2.2
1	D	30	VAL	2.2
1	D	81	THR	2.2
1	D	432	THR	2.2
1	C	352	GLN	2.2
1	B	44	GLY	2.1
1	A	310	THR	2.1
1	C	375	PRO	2.1
1	A	53	SER	2.1
1	A	52	ALA	2.0
1	C	158	ASN	2.0
1	B	40	VAL	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	90	GLY	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.