Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 08:17 PM EDT

PDB ID	:	2YVZ
Title	:	Crystal structure of magnesium transporter MgtE cytosolic domain, Mg2+-free form
Authors	:	Hattori, M.; Tanaka, Y.; Fukai, S.; Ishitani, R.; Nureki, O.
Deposited on	:	2007-04-18
Resolution	:	3.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (i)) were used in the production of this report:

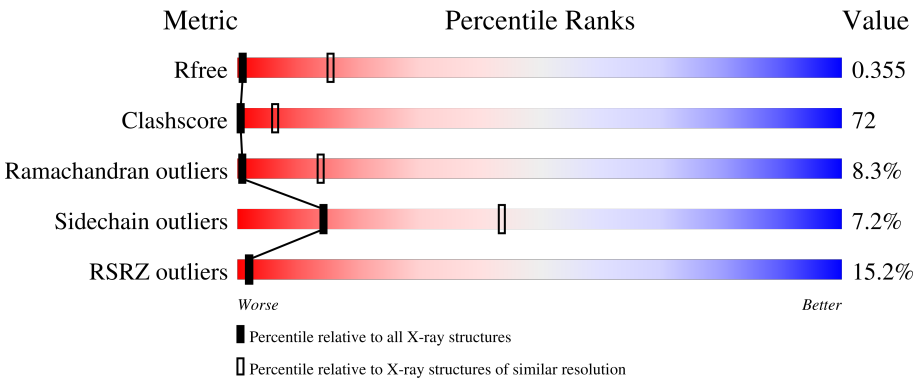
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 >=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 <=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	278	9%; 23%, 55%, 9%, •, 11%
1	B	278	18%; 24%, 55%, 9%, •, 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3982 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 Mg2+ transporter MgtE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	248	1991	1262	336	389	4	0	0	0
1	B	248	1991	1262	336	389	4	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

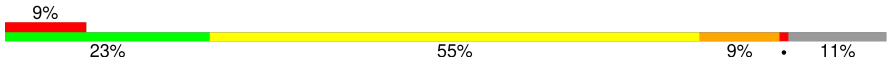
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q5SMG8
A	-1	SER	-	EXPRESSION TAG	UNP Q5SMG8
A	0	HIS	-	EXPRESSION TAG	UNP Q5SMG8
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q5SMG8
A	138	MSE	MET	MODIFIED RESIDUE	UNP Q5SMG8
A	149	MSE	MET	MODIFIED RESIDUE	UNP Q5SMG8
A	202	MSE	MET	MODIFIED RESIDUE	UNP Q5SMG8
A	222	MSE	MET	MODIFIED RESIDUE	UNP Q5SMG8
B	-2	GLY	-	EXPRESSION TAG	UNP Q5SMG8
B	-1	SER	-	EXPRESSION TAG	UNP Q5SMG8
B	0	HIS	-	EXPRESSION TAG	UNP Q5SMG8
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q5SMG8
B	138	MSE	MET	MODIFIED RESIDUE	UNP Q5SMG8
B	149	MSE	MET	MODIFIED RESIDUE	UNP Q5SMG8
B	202	MSE	MET	MODIFIED RESIDUE	UNP Q5SMG8
B	222	MSE	MET	MODIFIED RESIDUE	UNP Q5SMG8

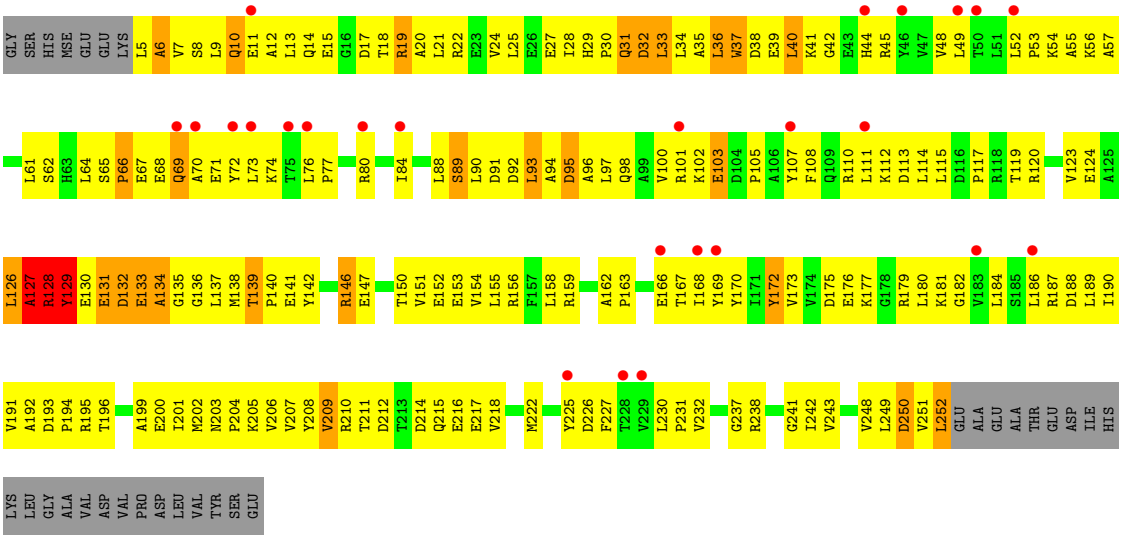
3 Residue-property plots (i)

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

- Molecule 1: Mg2+ transporter MgtE

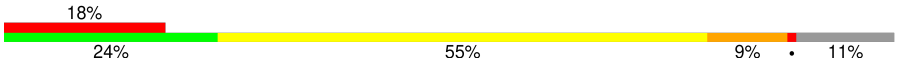
Chain A:

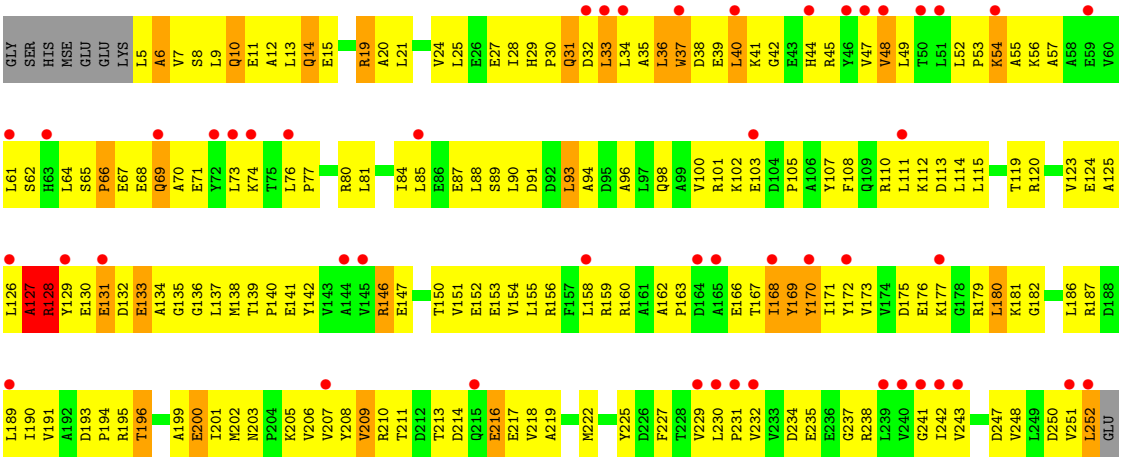




- Molecule 1: Mg2+ transporter MgtE

Chain B:





ALA
GLU
ALA
THR
GLU
ASP
ILE
HIS
LYS
LEU
GLY
ALA
VAL
ASP
VAL
PRO
ASP
LEU
VAL
TYR
SER
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.11Å 100.18Å 100.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.80 – 3.90 44.80 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.80-3.90) 99.4 (44.80-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 3.88Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.346 , 0.370 0.350 , 0.355	Depositor DCC
R_{free} test set	402 reflections (5.41%)	wwPDB-VP
Wilson B-factor (Å^2)	177.9	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 190.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.419 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3982	wwPDB-VP
Average B, all atoms (Å^2)	227.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]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	0.67	1/2018 (0.0%)	0.93	5/2738 (0.2%)
1	B	0.67	0/2018	0.86	1/2738 (0.0%)
All	All	0.67	1/4036 (0.0%)	0.90	6/5476 (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	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	GLU	CA-C	-5.45	1.38	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	GLU	N-CA-C	9.28	136.05	111.00
1	A	127	ALA	N-CA-C	7.94	132.44	111.00
1	B	127	ALA	N-CA-C	7.12	130.24	111.00
1	A	129	TYR	CA-CB-CG	-6.08	101.84	113.40
1	A	133	GLU	CA-C-N	-5.99	104.03	117.20
1	A	126	LEU	N-CA-C	5.29	125.28	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	TYR	Sidechain
1	A	172	TYR	Sidechain
1	B	170	TYR	Sidechain

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	1991	0	2006	327	0
1	B	1991	0	2006	280	0
All	All	3982	0	4012	578	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 72.

All (578) 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:130:GLU:HB3	1:A:133:GLU:HB2	1.27	1.17
1:A:133:GLU:O	1:A:135:GLY:N	1.78	1.16
1:B:13:LEU:HD11	1:B:21:LEU:HD13	1.29	1.14
1:B:113:ASP:HA	1:B:120:ARG:NH1	1.66	1.10
1:B:146:ARG:NH2	1:B:176:GLU:HA	1.67	1.10
1:B:113:ASP:HA	1:B:120:ARG:HH12	1.14	1.03
1:B:9:LEU:HD11	1:B:21:LEU:HA	1.38	1.02
1:A:113:ASP:HA	1:A:120:ARG:HH12	1.26	1.01
1:A:203:ASN:OD1	1:A:205:LYS:HE3	1.65	0.97
1:A:71:GLU:HA	1:A:74:LYS:HE2	1.45	0.95
1:B:24:VAL:O	1:B:28:ILE:HB	1.67	0.95
1:B:76:LEU:HD23	1:B:77:PRO:HD2	1.50	0.94
1:A:36:LEU:HD23	1:A:36:LEU:H	1.33	0.93
1:A:24:VAL:O	1:A:28:ILE:HB	1.69	0.91
1:A:187:ARG:HG3	1:B:168:ILE:HD11	1.52	0.91
1:A:120:ARG:O	1:A:124:GLU:HG3	1.70	0.91
1:B:77:PRO:HG2	1:B:80:ARG:CB	2.04	0.88
1:A:113:ASP:HA	1:A:120:ARG:NH1	1.87	0.88
1:A:130:GLU:CB	1:A:133:GLU:HB2	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:LEU:HD23	1:B:36:LEU:H	1.38	0.88
1:B:5:LEU:HD22	1:B:24:VAL:HG13	1.56	0.87
1:B:146:ARG:HH22	1:B:176:GLU:HA	1.39	0.86
1:B:120:ARG:O	1:B:124:GLU:HG3	1.76	0.86
1:B:135:GLY:HA2	1:B:138:MSE:HE3	1.57	0.85
1:A:70:ALA:O	1:A:74:LYS:HG3	1.76	0.85
1:B:124:GLU:O	1:B:128:ARG:NH1	2.10	0.85
1:A:131:GLU:C	1:A:133:GLU:OE1	2.15	0.84
1:A:184:LEU:HD21	1:A:189:LEU:HD21	1.57	0.84
1:A:250:ASP:O	1:A:252:LEU:HD13	1.77	0.84
1:A:119:THR:O	1:A:123:VAL:HG23	1.78	0.84
1:B:77:PRO:HG2	1:B:80:ARG:HB3	1.60	0.83
1:A:5:LEU:HD22	1:A:24:VAL:HG13	1.60	0.83
1:A:134:ALA:HB3	1:A:211:THR:O	1.79	0.83
1:B:162:ALA:HB3	1:B:163:PRO:HD3	1.61	0.83
1:A:77:PRO:HG2	1:A:80:ARG:CB	2.09	0.83
1:B:19:ARG:HG3	1:B:20:ALA:H	1.43	0.82
1:A:162:ALA:HB3	1:A:163:PRO:HD3	1.60	0.82
1:A:61:LEU:HD12	1:A:64:LEU:HD12	1.62	0.81
1:A:9:LEU:HD11	1:A:21:LEU:HD12	1.62	0.81
1:A:52:LEU:HD23	1:A:57:ALA:HA	1.63	0.80
1:A:187:ARG:NH2	1:B:166:GLU:O	2.15	0.79
1:B:76:LEU:CD2	1:B:77:PRO:HD2	2.13	0.79
1:A:193:ASP:OD2	1:A:195:ARG:HB2	1.82	0.79
1:B:52:LEU:HD23	1:B:57:ALA:HA	1.65	0.79
1:A:128:ARG:HH21	1:A:136:GLY:HA2	1.47	0.79
1:B:162:ALA:N	1:B:163:PRO:CD	2.44	0.79
1:A:162:ALA:N	1:A:163:PRO:CD	2.47	0.78
1:A:179:ARG:HA	1:A:238:ARG:HA	1.64	0.78
1:B:112:LYS:O	1:B:120:ARG:HG3	1.84	0.78
1:A:190:ILE:HD12	1:A:190:ILE:H	1.49	0.78
1:B:13:LEU:HD23	1:B:44:HIS:ND1	1.99	0.77
1:A:132:ASP:HB3	1:A:215:GLN:NE2	2.00	0.77
1:A:112:LYS:HE3	1:A:124:GLU:HG2	1.65	0.77
1:B:179:ARG:HA	1:B:238:ARG:HA	1.67	0.77
1:B:136:GLY:O	1:B:137:LEU:HD23	1.84	0.76
1:A:207:VAL:HG11	1:A:225:TYR:CE2	2.21	0.76
1:B:193:ASP:OD2	1:B:195:ARG:HG3	1.86	0.76
1:B:29:HIS:CE1	1:B:31:GLN:HB2	2.20	0.76
1:B:66:PRO:HG2	1:B:67:GLU:OE2	1.85	0.76
1:B:207:VAL:HG21	1:B:227:PHE:HE1	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:TRP:O	1:A:39:GLU:N	2.20	0.75
1:B:172:TYR:CE2	1:B:231:PRO:HB3	2.22	0.75
1:A:132:ASP:N	1:A:133:GLU:OE1	2.20	0.74
1:A:36:LEU:HD23	1:A:36:LEU:N	2.02	0.74
1:A:77:PRO:HG2	1:A:80:ARG:HB2	1.68	0.74
1:B:115:LEU:HD23	1:B:120:ARG:HA	1.69	0.74
1:A:7:VAL:HG22	1:A:10:GLN:NE2	2.02	0.74
1:B:107:TYR:CE2	1:B:111:LEU:HD11	2.22	0.74
1:B:37:TRP:O	1:B:39:GLU:N	2.21	0.73
1:A:37:TRP:HE1	1:A:45:ARG:NH1	1.85	0.73
1:A:180:LEU:HD23	1:A:181:LYS:N	2.02	0.73
1:B:150:THR:O	1:B:154:VAL:HG23	1.89	0.73
1:B:208:TYR:CD2	1:B:209:VAL:N	2.56	0.73
1:A:162:ALA:CB	1:B:191:VAL:HG11	2.19	0.72
1:A:48:VAL:HG23	1:A:49:LEU:H	1.52	0.72
1:A:105:PRO:O	1:A:108:PHE:HB3	1.89	0.72
1:A:128:ARG:NH2	1:A:136:GLY:HA2	2.04	0.72
1:A:88:LEU:HD23	1:A:93:LEU:HA	1.69	0.72
1:A:162:ALA:HB1	1:B:191:VAL:HG11	1.72	0.72
1:B:94:ALA:HB2	1:B:126:LEU:HD23	1.72	0.71
1:B:110:ARG:O	1:B:114:LEU:HG	1.90	0.71
1:A:151:VAL:HB	1:A:194:PRO:HA	1.73	0.71
1:B:153:GLU:HG2	1:B:156:ARG:HH22	1.55	0.71
1:A:138:MSE:HE1	1:A:211:THR:HG22	1.73	0.71
1:A:135:GLY:HA2	1:A:138:MSE:HE2	1.72	0.71
1:B:77:PRO:HG2	1:B:80:ARG:HB2	1.71	0.71
1:B:142:TYR:HB3	1:B:242:ILE:HG21	1.71	0.71
1:B:151:VAL:HB	1:B:194:PRO:HA	1.72	0.70
1:A:128:ARG:HE	1:A:135:GLY:C	1.95	0.70
1:A:168:ILE:O	1:A:186:LEU:HD13	1.91	0.70
1:A:131:GLU:CA	1:A:133:GLU:OE1	2.39	0.70
1:A:130:GLU:HB3	1:A:133:GLU:CB	2.16	0.70
1:A:142:TYR:HB3	1:A:242:ILE:HG21	1.71	0.70
1:B:9:LEU:CD1	1:B:21:LEU:HA	2.18	0.70
1:B:13:LEU:CD1	1:B:21:LEU:HD13	2.15	0.70
1:A:166:GLU:O	1:B:187:ARG:NH2	2.21	0.70
1:B:105:PRO:O	1:B:108:PHE:HB3	1.92	0.69
1:A:77:PRO:HG2	1:A:80:ARG:HB3	1.73	0.69
1:A:133:GLU:C	1:A:135:GLY:N	2.45	0.69
1:A:167:THR:OG1	1:A:169:TYR:HB2	1.93	0.69
1:A:52:LEU:HD23	1:A:57:ALA:CA	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:HD23	1:B:57:ALA:CA	2.23	0.69
1:B:167:THR:OG1	1:B:169:TYR:HB2	1.92	0.69
1:A:130:GLU:CD	1:A:212:ASP:HA	2.12	0.68
1:B:171:ILE:N	1:B:171:ILE:HD12	2.08	0.68
1:A:188:ASP:O	1:A:191:VAL:HG22	1.93	0.68
1:A:101:ARG:NH2	1:A:129:TYR:O	2.27	0.68
1:A:69:GLN:O	1:A:73:LEU:HG	1.93	0.68
1:B:5:LEU:CD2	1:B:24:VAL:HG13	2.24	0.68
1:A:36:LEU:H	1:A:36:LEU:CD2	2.04	0.68
1:B:101:ARG:HH21	1:B:130:GLU:HB2	1.59	0.68
1:B:139:THR:O	1:B:141:GLU:N	2.26	0.68
1:A:76:LEU:HD23	1:A:77:PRO:HD2	1.74	0.68
1:A:187:ARG:NH2	1:B:167:THR:HA	2.09	0.68
1:B:180:LEU:HD23	1:B:181:LYS:N	2.09	0.68
1:A:112:LYS:O	1:A:120:ARG:HG3	1.94	0.67
1:A:128:ARG:HH21	1:A:135:GLY:C	1.98	0.67
1:B:13:LEU:HD23	1:B:44:HIS:CE1	2.30	0.67
1:A:133:GLU:OE1	1:A:133:GLU:N	2.27	0.67
1:A:135:GLY:HA2	1:A:138:MSE:CE	2.24	0.67
1:A:202:MSE:O	1:A:202:MSE:HG3	1.94	0.67
1:A:13:LEU:HD23	1:A:44:HIS:ND1	2.10	0.67
1:A:111:LEU:O	1:A:115:LEU:HD13	1.95	0.67
1:A:218:VAL:O	1:A:222:MSE:HE2	1.95	0.67
1:A:5:LEU:CD2	1:A:24:VAL:HG13	2.25	0.66
1:B:65:SER:OG	1:B:68:GLU:OE1	2.13	0.66
1:A:136:GLY:O	1:A:137:LEU:HD23	1.94	0.66
1:A:139:THR:O	1:A:141:GLU:N	2.28	0.66
1:B:135:GLY:HA2	1:B:138:MSE:CE	2.25	0.66
1:A:112:LYS:O	1:A:115:LEU:HB2	1.96	0.66
1:A:5:LEU:HD13	1:A:27:GLU:O	1.97	0.65
1:B:5:LEU:HA	1:B:8:SER:HB3	1.78	0.65
1:B:70:ALA:HB1	1:B:100:VAL:HG13	1.78	0.65
1:A:190:ILE:HG23	1:B:155:LEU:HD22	1.78	0.65
1:A:107:TYR:CE2	1:A:111:LEU:HD11	2.31	0.65
1:A:66:PRO:HG2	1:A:67:GLU:OE2	1.97	0.65
1:A:76:LEU:CD2	1:A:77:PRO:HD2	2.27	0.65
1:B:210:ARG:HH11	1:B:235:GLU:HA	1.61	0.65
1:B:203:ASN:OD1	1:B:205:LYS:HE3	1.96	0.64
1:A:172:TYR:CE2	1:A:231:PRO:HB3	2.32	0.64
1:A:142:TYR:HB3	1:A:242:ILE:HD13	1.78	0.64
1:A:180:LEU:HD23	1:A:182:GLY:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ILE:HG21	1:B:158:LEU:HD23	1.80	0.64
1:A:203:ASN:OD1	1:A:205:LYS:HB2	1.98	0.64
1:B:7:VAL:HG13	1:B:10:GLN:NE2	2.12	0.63
1:B:61:LEU:HD12	1:B:64:LEU:HD12	1.80	0.63
1:B:81:LEU:O	1:B:85:LEU:HG	1.97	0.63
1:B:19:ARG:HG3	1:B:20:ALA:N	2.13	0.63
1:A:249:LEU:O	1:A:249:LEU:HD23	1.98	0.63
1:A:61:LEU:CD1	1:A:64:LEU:HD12	2.28	0.63
1:B:77:PRO:O	1:B:81:LEU:HG	1.98	0.63
1:B:242:ILE:HG13	1:B:242:ILE:O	1.97	0.63
1:A:169:TYR:CE2	1:B:187:ARG:HB2	2.34	0.63
1:A:146:ARG:NH2	1:A:176:GLU:HA	2.13	0.63
1:B:5:LEU:HB3	1:B:24:VAL:HG13	1.80	0.63
1:B:125:ALA:HA	1:B:128:ARG:NH1	2.14	0.62
1:B:48:VAL:HG23	1:B:49:LEU:H	1.63	0.62
1:B:107:TYR:CD2	1:B:111:LEU:HD11	2.34	0.62
1:A:128:ARG:HH21	1:A:136:GLY:CA	2.13	0.62
1:B:36:LEU:H	1:B:36:LEU:CD2	2.10	0.62
1:A:133:GLU:O	1:A:135:GLY:CA	2.48	0.62
1:B:53:PRO:O	1:B:55:ALA:N	2.32	0.62
1:A:132:ASP:OD2	1:A:215:GLN:NE2	2.24	0.62
1:A:190:ILE:HD12	1:A:190:ILE:N	2.13	0.62
1:B:250:ASP:C	1:B:252:LEU:H	2.03	0.62
1:A:128:ARG:HE	1:A:135:GLY:CA	2.13	0.62
1:A:29:HIS:ND1	1:A:30:PRO:HD2	2.15	0.61
1:B:180:LEU:HD23	1:B:182:GLY:H	1.64	0.61
1:A:9:LEU:HD13	1:A:24:VAL:HB	1.82	0.61
1:A:133:GLU:OE2	1:A:215:GLN:HB3	2.00	0.61
1:A:128:ARG:NH2	1:A:135:GLY:O	2.32	0.61
1:A:53:PRO:O	1:A:55:ALA:N	2.34	0.61
1:A:167:THR:HA	1:B:187:ARG:CZ	2.30	0.61
1:B:172:TYR:OH	1:B:231:PRO:HD3	2.00	0.61
1:A:248:VAL:HA	1:A:251:VAL:HG22	1.83	0.61
1:A:208:TYR:CD2	1:A:209:VAL:N	2.69	0.61
1:A:210:ARG:HB3	1:A:212:ASP:OD1	1.99	0.61
1:B:67:GLU:H	1:B:67:GLU:CD	2.03	0.61
1:A:25:LEU:HA	1:A:28:ILE:CG2	2.31	0.61
1:B:147:GLU:OE1	1:B:181:LYS:HG3	2.01	0.61
1:A:222:MSE:HE1	1:A:248:VAL:HG21	1.82	0.60
1:A:115:LEU:HD23	1:A:120:ARG:HA	1.83	0.60
1:A:133:GLU:O	1:A:134:ALA:C	2.40	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:O	1:B:93:LEU:HB3	2.00	0.60
1:A:147:GLU:OE1	1:A:181:LYS:HG3	2.02	0.60
1:B:36:LEU:HD23	1:B:36:LEU:N	2.11	0.60
1:A:67:GLU:CD	1:A:67:GLU:H	2.05	0.60
1:B:80:ARG:O	1:B:84:ILE:HG12	2.02	0.60
1:B:175:ASP:O	1:B:176:GLU:C	2.37	0.60
1:A:175:ASP:O	1:A:176:GLU:C	2.38	0.60
1:B:207:VAL:HG23	1:B:230:LEU:HD11	1.83	0.60
1:A:190:ILE:HD11	1:B:190:ILE:HD11	1.84	0.60
1:A:180:LEU:HD23	1:A:182:GLY:N	2.17	0.60
1:B:89:SER:O	1:B:93:LEU:HB2	2.02	0.59
1:B:173:VAL:HG21	1:B:202:MSE:SE	2.52	0.59
1:A:13:LEU:HD23	1:A:44:HIS:CE1	2.37	0.59
1:A:7:VAL:HG12	1:A:7:VAL:O	2.01	0.59
1:A:105:PRO:O	1:A:108:PHE:N	2.35	0.59
1:A:186:LEU:HD11	1:B:190:ILE:HD12	1.82	0.59
1:B:203:ASN:ND2	1:B:205:LYS:HE3	2.17	0.59
1:B:5:LEU:HD13	1:B:27:GLU:HG3	1.84	0.59
1:B:5:LEU:HB3	1:B:24:VAL:CG1	2.32	0.58
1:A:7:VAL:HA	1:A:10:GLN:HE21	1.67	0.58
1:A:94:ALA:O	1:A:98:GLN:HG3	2.04	0.58
1:A:107:TYR:CD2	1:A:111:LEU:HD11	2.38	0.58
1:B:105:PRO:O	1:B:108:PHE:N	2.36	0.58
1:A:110:ARG:O	1:A:114:LEU:HG	2.03	0.58
1:A:19:ARG:CD	1:A:20:ALA:N	2.67	0.58
1:A:203:ASN:ND2	1:A:205:LYS:O	2.36	0.58
1:A:217:GLU:OE1	1:A:217:GLU:HA	2.04	0.58
1:A:13:LEU:O	1:A:15:GLU:N	2.36	0.58
1:A:191:VAL:HG23	1:A:192:ALA:N	2.18	0.58
1:A:250:ASP:C	1:A:252:LEU:H	2.07	0.58
1:B:168:ILE:O	1:B:186:LEU:HD13	2.04	0.58
1:B:119:THR:O	1:B:123:VAL:HG23	2.04	0.57
1:A:207:VAL:HG23	1:A:207:VAL:O	2.02	0.57
1:B:13:LEU:O	1:B:15:GLU:N	2.37	0.57
1:B:168:ILE:O	1:B:171:ILE:HD11	2.04	0.57
1:B:203:ASN:OD1	1:B:205:LYS:CE	2.53	0.57
1:B:54:LYS:O	1:B:87:GLU:HG3	2.05	0.57
1:A:5:LEU:HB3	1:A:24:VAL:HG13	1.86	0.57
1:B:9:LEU:HD12	1:B:12:ALA:HB3	1.85	0.57
1:A:13:LEU:C	1:A:15:GLU:H	2.06	0.57
1:A:128:ARG:NE	1:A:135:GLY:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:TYR:N	1:B:225:TYR:CD1	2.69	0.57
1:A:105:PRO:O	1:A:108:PHE:CB	2.53	0.57
1:A:53:PRO:HG2	1:A:56:LYS:HD2	1.86	0.57
1:B:139:THR:C	1:B:141:GLU:H	2.08	0.56
1:A:13:LEU:CD1	1:A:21:LEU:HD13	2.35	0.56
1:A:107:TYR:CZ	1:A:111:LEU:HD21	2.40	0.56
1:A:131:GLU:N	1:A:133:GLU:OE1	2.39	0.56
1:B:217:GLU:HA	1:B:217:GLU:OE1	2.05	0.56
1:A:168:ILE:HD11	1:B:187:ARG:HG3	1.87	0.56
1:B:5:LEU:CD1	1:B:27:GLU:HG3	2.36	0.56
1:B:218:VAL:HG12	1:B:218:VAL:O	2.04	0.56
1:A:132:ASP:OD2	1:A:251:VAL:HG12	2.05	0.56
1:B:41:LYS:O	1:B:42:GLY:C	2.44	0.56
1:B:160:ARG:NH1	1:B:160:ARG:HG3	2.21	0.56
1:B:203:ASN:CG	1:B:205:LYS:HE3	2.26	0.56
1:B:247:ASP:O	1:B:251:VAL:HG13	2.05	0.56
1:A:41:LYS:O	1:A:42:GLY:C	2.42	0.56
1:A:90:LEU:O	1:A:93:LEU:CB	2.54	0.56
1:B:210:ARG:NH1	1:B:235:GLU:HA	2.21	0.56
1:A:202:MSE:HE3	1:A:204:PRO:HA	1.87	0.55
1:B:53:PRO:CG	1:B:56:LYS:HD2	2.35	0.55
1:B:13:LEU:C	1:B:15:GLU:H	2.09	0.55
1:A:91:ASP:O	1:A:94:ALA:HB3	2.06	0.55
1:B:107:TYR:CZ	1:B:111:LEU:HD21	2.41	0.55
1:B:207:VAL:HG21	1:B:227:PHE:CE1	2.37	0.55
1:A:62:SER:HA	1:A:69:GLN:HE22	1.70	0.55
1:A:9:LEU:HD11	1:A:21:LEU:CD1	2.35	0.55
1:A:53:PRO:CG	1:A:56:LYS:HD2	2.37	0.55
1:A:202:MSE:HE3	1:A:204:PRO:CA	2.37	0.54
1:A:94:ALA:HB2	1:A:126:LEU:HD23	1.90	0.54
1:A:105:PRO:HA	1:A:108:PHE:HB2	1.89	0.54
1:A:133:GLU:OE2	1:A:215:GLN:CB	2.55	0.54
1:B:53:PRO:HG2	1:B:56:LYS:HG3	1.89	0.54
1:B:88:LEU:HD23	1:B:93:LEU:HA	1.87	0.54
1:A:48:VAL:O	1:A:52:LEU:HB2	2.08	0.54
1:A:89:SER:O	1:A:93:LEU:HB2	2.07	0.54
1:A:186:LEU:O	1:A:190:ILE:CD1	2.55	0.54
1:B:13:LEU:HD12	1:B:13:LEU:N	2.22	0.54
1:B:168:ILE:HD13	1:B:168:ILE:H	1.73	0.54
1:B:203:ASN:OD1	1:B:205:LYS:HB2	2.08	0.54
1:A:25:LEU:O	1:A:28:ILE:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ALA:HB2	1:B:191:VAL:CG1	2.38	0.54
1:A:95:ASP:OD1	1:A:95:ASP:N	2.41	0.54
1:B:207:VAL:HG23	1:B:207:VAL:O	2.06	0.54
1:A:17:ASP:OD1	1:A:19:ARG:HG3	2.08	0.54
1:A:146:ARG:HH11	1:A:146:ARG:HB3	1.72	0.54
1:A:147:GLU:HB3	1:A:173:VAL:CG1	2.38	0.54
1:A:5:LEU:HA	1:A:8:SER:HB3	1.89	0.54
1:A:162:ALA:CB	1:B:191:VAL:CG1	2.84	0.54
1:A:180:LEU:HD21	1:A:206:VAL:HG11	1.89	0.54
1:B:193:ASP:CG	1:B:194:PRO:HD2	2.28	0.54
1:A:142:TYR:HB3	1:A:242:ILE:CG2	2.36	0.53
1:A:62:SER:HA	1:A:69:GLN:NE2	2.23	0.53
1:A:19:ARG:HD3	1:A:20:ALA:N	2.24	0.53
1:A:131:GLU:O	1:A:132:ASP:HB2	2.08	0.53
1:A:187:ARG:NH1	1:B:167:THR:OG1	2.42	0.53
1:B:53:PRO:HG2	1:B:56:LYS:CG	2.39	0.53
1:B:71:GLU:HA	1:B:74:LYS:HE2	1.90	0.53
1:B:169:TYR:C	1:B:170:TYR:CD1	2.82	0.53
1:A:130:GLU:C	1:A:132:ASP:H	2.12	0.53
1:A:130:GLU:OE1	1:A:212:ASP:O	2.27	0.53
1:A:89:SER:HB3	1:A:91:ASP:OD1	2.09	0.52
1:A:132:ASP:HB3	1:A:215:GLN:CD	2.30	0.52
1:A:139:THR:C	1:A:141:GLU:H	2.11	0.52
1:B:31:GLN:O	1:B:33:LEU:N	2.43	0.52
1:B:48:VAL:O	1:B:52:LEU:HB2	2.10	0.52
1:A:207:VAL:HG11	1:A:225:TYR:CZ	2.43	0.52
1:A:6:ALA:C	1:A:8:SER:H	2.13	0.52
1:A:232:VAL:CG2	1:A:243:VAL:HG23	2.39	0.52
1:B:139:THR:O	1:B:139:THR:HG23	2.09	0.52
1:A:130:GLU:CB	1:A:133:GLU:CB	2.84	0.52
1:B:162:ALA:N	1:B:163:PRO:HD3	2.22	0.52
1:B:142:TYR:HB3	1:B:242:ILE:CG2	2.39	0.52
1:B:134:ALA:HB3	1:B:211:THR:O	2.10	0.52
1:B:138:MSE:HA	1:B:242:ILE:O	2.10	0.52
1:A:37:TRP:NE1	1:A:45:ARG:NH1	2.57	0.51
1:A:162:ALA:HB2	1:B:191:VAL:HG12	1.91	0.51
1:A:41:LYS:HB2	1:A:44:HIS:HD2	1.75	0.51
1:B:31:GLN:C	1:B:33:LEU:N	2.60	0.51
1:B:232:VAL:CG2	1:B:243:VAL:HG23	2.39	0.51
1:B:24:VAL:HG12	1:B:28:ILE:HD13	1.92	0.51
1:B:91:ASP:O	1:B:94:ALA:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ALA:CB	1:A:163:PRO:HD3	2.30	0.51
1:B:147:GLU:HB3	1:B:173:VAL:CG1	2.40	0.51
1:A:162:ALA:N	1:A:163:PRO:HD3	2.23	0.51
1:B:13:LEU:CD1	1:B:13:LEU:N	2.74	0.51
1:B:101:ARG:O	1:B:103:GLU:N	2.43	0.51
1:B:250:ASP:C	1:B:252:LEU:N	2.64	0.51
1:A:177:LYS:NZ	1:A:179:ARG:HH22	2.09	0.51
1:B:33:LEU:C	1:B:35:ALA:H	2.14	0.51
1:B:162:ALA:N	1:B:163:PRO:HD2	2.25	0.50
1:A:31:GLN:C	1:A:33:LEU:N	2.62	0.50
1:A:184:LEU:CD2	1:A:189:LEU:HD21	2.36	0.50
1:B:49:LEU:HD23	1:B:57:ALA:HA	1.93	0.50
1:A:65:SER:OG	1:A:68:GLU:OE1	2.29	0.50
1:A:177:LYS:HZ2	1:A:179:ARG:NH2	2.09	0.50
1:B:180:LEU:CD2	1:B:182:GLY:H	2.24	0.50
1:A:138:MSE:HA	1:A:242:ILE:O	2.12	0.50
1:A:187:ARG:CZ	1:B:167:THR:HA	2.41	0.50
1:A:214:ASP:OD2	1:A:216:GLU:HB2	2.12	0.50
1:B:9:LEU:HD11	1:B:21:LEU:HD12	1.94	0.50
1:B:115:LEU:HB3	1:B:120:ARG:HB2	1.94	0.50
1:B:167:THR:HG1	1:B:169:TYR:HB2	1.77	0.50
1:A:31:GLN:O	1:A:33:LEU:N	2.45	0.50
1:B:12:ALA:C	1:B:13:LEU:HD12	2.30	0.50
1:B:62:SER:HA	1:B:69:GLN:NE2	2.26	0.50
1:A:19:ARG:HG3	1:A:20:ALA:H	1.77	0.50
1:A:19:ARG:CG	1:A:20:ALA:H	2.24	0.50
1:A:177:LYS:HZ2	1:A:179:ARG:HH22	1.60	0.49
1:A:187:ARG:HG3	1:B:168:ILE:CD1	2.32	0.49
1:A:203:ASN:HD21	1:A:205:LYS:HB2	1.77	0.49
1:B:70:ALA:O	1:B:74:LYS:HG3	2.12	0.49
1:A:158:LEU:O	1:A:162:ALA:HB2	2.12	0.49
1:B:101:ARG:NH2	1:B:130:GLU:HB2	2.27	0.49
1:B:105:PRO:O	1:B:108:PHE:CB	2.59	0.49
1:B:180:LEU:CD2	1:B:182:GLY:N	2.75	0.49
1:B:196:THR:HG22	1:B:200:GLU:HB2	1.94	0.49
1:B:199:ALA:O	1:B:201:ILE:N	2.45	0.49
1:A:130:GLU:CG	1:A:212:ASP:HA	2.42	0.49
1:A:184:LEU:HD21	1:A:189:LEU:CD2	2.35	0.49
1:A:41:LYS:HB2	1:A:44:HIS:CD2	2.48	0.49
1:A:88:LEU:HD23	1:A:92:ASP:O	2.13	0.49
1:A:218:VAL:O	1:A:218:VAL:HG12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:TYR:HD2	1:B:209:VAL:H	1.59	0.49
1:B:179:ARG:CB	1:B:237:GLY:O	2.61	0.49
1:B:180:LEU:HD21	1:B:206:VAL:HG11	1.95	0.49
1:A:132:ASP:CB	1:A:215:GLN:NE2	2.73	0.49
1:A:101:ARG:O	1:A:103:GLU:N	2.45	0.49
1:A:133:GLU:N	1:A:133:GLU:CD	2.66	0.49
1:A:138:MSE:HE1	1:A:211:THR:CG2	2.42	0.49
1:A:250:ASP:C	1:A:252:LEU:N	2.66	0.49
1:B:33:LEU:O	1:B:35:ALA:N	2.45	0.49
1:B:132:ASP:O	1:B:133:GLU:CB	2.61	0.49
1:A:129:TYR:C	1:A:129:TYR:CD2	2.85	0.48
1:B:115:LEU:HD23	1:B:120:ARG:CA	2.42	0.48
1:B:222:MSE:HE1	1:B:248:VAL:HG21	1.94	0.48
1:A:107:TYR:CE2	1:A:111:LEU:HD21	2.48	0.48
1:B:214:ASP:OD2	1:B:216:GLU:HB2	2.13	0.48
1:A:199:ALA:O	1:A:201:ILE:N	2.46	0.48
1:B:7:VAL:HA	1:B:10:GLN:HE21	1.77	0.48
1:B:158:LEU:O	1:B:162:ALA:HB2	2.13	0.48
1:B:162:ALA:CB	1:B:163:PRO:HD3	2.30	0.48
1:A:5:LEU:CD1	1:A:27:GLU:O	2.61	0.48
1:A:25:LEU:HA	1:A:28:ILE:HG21	1.95	0.48
1:B:234:ASP:OD2	1:B:238:ARG:HB2	2.14	0.48
1:B:210:ARG:HB2	1:B:213:THR:OG1	2.13	0.48
1:A:135:GLY:CA	1:A:138:MSE:HE2	2.41	0.48
1:A:226:ASP:N	1:A:226:ASP:OD1	2.47	0.48
1:A:191:VAL:HA	1:B:159:ARG:HG2	1.95	0.48
1:B:9:LEU:C	1:B:11:GLU:H	2.16	0.48
1:B:94:ALA:CB	1:B:126:LEU:HD23	2.42	0.48
1:B:203:ASN:HD21	1:B:205:LYS:HE3	1.77	0.48
1:A:33:LEU:C	1:A:35:ALA:H	2.17	0.48
1:A:207:VAL:CG2	1:A:227:PHE:HE1	2.27	0.48
1:B:207:VAL:CG2	1:B:227:PHE:HE1	2.24	0.48
1:A:18:THR:HG22	1:A:22:ARG:HE	1.79	0.48
1:A:19:ARG:CG	1:A:20:ALA:N	2.77	0.48
1:A:101:ARG:HH22	1:A:129:TYR:N	2.12	0.48
1:A:180:LEU:CD2	1:A:182:GLY:N	2.77	0.48
1:B:52:LEU:HD12	1:B:53:PRO:HD2	1.96	0.48
1:B:160:ARG:HG3	1:B:160:ARG:HH11	1.77	0.48
1:A:9:LEU:C	1:A:11:GLU:H	2.17	0.47
1:B:128:ARG:HG3	1:B:129:TYR:CE2	2.49	0.47
1:B:6:ALA:C	1:B:8:SER:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:C	1:A:15:GLU:N	2.67	0.47
1:A:138:MSE:SE	1:A:241:GLY:HA3	2.64	0.47
1:A:193:ASP:OD1	1:A:194:PRO:HD2	2.14	0.47
1:B:138:MSE:HE1	1:B:211:THR:HG22	1.96	0.47
1:B:234:ASP:OD1	1:B:235:GLU:N	2.48	0.47
1:A:29:HIS:CE1	1:A:31:GLN:HB2	2.50	0.47
1:A:133:GLU:OE2	1:A:215:GLN:HG2	2.15	0.47
1:A:146:ARG:HH11	1:A:146:ARG:CG	2.27	0.47
1:A:130:GLU:HG3	1:A:212:ASP:HA	1.95	0.47
1:A:187:ARG:CG	1:B:168:ILE:HD11	2.36	0.47
1:B:19:ARG:CG	1:B:20:ALA:N	2.78	0.47
1:A:153:GLU:HA	1:A:156:ARG:NH2	2.29	0.47
1:B:153:GLU:HA	1:B:156:ARG:NH2	2.30	0.47
1:A:172:TYR:N	1:A:172:TYR:CD1	2.83	0.47
1:A:227:PHE:HD1	1:A:230:LEU:CD1	2.27	0.47
1:B:202:MSE:O	1:B:202:MSE:HG3	2.15	0.47
1:A:80:ARG:O	1:A:84:ILE:HG12	2.14	0.46
1:A:33:LEU:O	1:A:35:ALA:N	2.48	0.46
1:A:97:LEU:HD12	1:A:123:VAL:HG11	1.97	0.46
1:A:232:VAL:HG21	1:A:243:VAL:HG23	1.97	0.46
1:B:150:THR:C	1:B:152:GLU:N	2.68	0.46
1:B:173:VAL:HG11	1:B:202:MSE:SE	2.65	0.46
1:A:128:ARG:NH2	1:A:135:GLY:C	2.68	0.46
1:A:168:ILE:HD11	1:B:187:ARG:HA	1.96	0.46
1:A:37:TRP:NE1	1:A:45:ARG:CZ	2.79	0.46
1:A:37:TRP:C	1:A:39:GLU:H	2.18	0.46
1:B:31:GLN:C	1:B:33:LEU:H	2.18	0.46
1:A:29:HIS:HB3	1:A:32:ASP:OD2	2.16	0.46
1:A:48:VAL:HG23	1:A:49:LEU:N	2.27	0.46
1:A:146:ARG:HH22	1:A:176:GLU:HA	1.79	0.46
1:A:207:VAL:HG11	1:A:225:TYR:OH	2.16	0.46
1:A:133:GLU:OE2	1:A:215:GLN:CG	2.64	0.46
1:B:13:LEU:C	1:B:15:GLU:N	2.68	0.46
1:A:179:ARG:HB2	1:A:237:GLY:O	2.16	0.46
1:A:208:TYR:OH	1:A:210:ARG:NH2	2.49	0.46
1:A:150:THR:OG1	1:A:152:GLU:HB3	2.16	0.46
1:B:171:ILE:N	1:B:171:ILE:CD1	2.77	0.46
1:B:172:TYR:HE2	1:B:231:PRO:HG3	1.81	0.46
1:B:105:PRO:HA	1:B:108:PHE:HB2	1.98	0.45
1:B:138:MSE:SE	1:B:241:GLY:HA3	2.66	0.45
1:B:206:VAL:HG13	1:B:206:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:HD23	1:A:180:LEU:C	2.37	0.45
1:A:193:ASP:OD2	1:A:195:ARG:CB	2.60	0.45
1:B:29:HIS:ND1	1:B:31:GLN:HB2	2.29	0.45
1:B:229:VAL:HG12	1:B:230:LEU:N	2.31	0.45
1:A:167:THR:HA	1:B:187:ARG:NH2	2.31	0.45
1:B:10:GLN:O	1:B:14:GLN:OE1	2.34	0.45
1:B:37:TRP:NE1	1:B:45:ARG:NH1	2.64	0.45
1:B:25:LEU:HA	1:B:28:ILE:CG2	2.46	0.45
1:B:130:GLU:HG3	1:B:131:GLU:N	2.32	0.45
1:A:71:GLU:O	1:A:71:GLU:HG2	2.16	0.45
1:B:70:ALA:HB2	1:B:100:VAL:HG22	1.99	0.45
1:A:128:ARG:NE	1:A:135:GLY:C	2.68	0.45
1:A:90:LEU:HA	1:A:93:LEU:HB2	1.98	0.45
1:A:203:ASN:ND2	1:A:205:LYS:HB2	2.31	0.45
1:B:37:TRP:C	1:B:39:GLU:H	2.20	0.45
1:A:88:LEU:HD23	1:A:93:LEU:CA	2.44	0.44
1:A:5:LEU:CD1	1:A:27:GLU:HG3	2.48	0.44
1:A:101:ARG:HH21	1:A:129:TYR:HB3	1.82	0.44
1:B:10:GLN:O	1:B:14:GLN:CD	2.55	0.44
1:A:158:LEU:HD23	1:B:190:ILE:HG21	1.97	0.44
1:A:215:GLN:NE2	1:A:251:VAL:CG1	2.80	0.44
1:B:70:ALA:HB2	1:B:100:VAL:HA	1.99	0.44
1:B:101:ARG:HH21	1:B:130:GLU:CB	2.26	0.44
1:A:190:ILE:H	1:A:190:ILE:CD1	2.24	0.44
1:B:73:LEU:O	1:B:107:TYR:OH	2.26	0.44
1:B:177:LYS:HZ2	1:B:179:ARG:NH2	2.16	0.44
1:B:218:VAL:O	1:B:222:MSE:HE2	2.17	0.44
1:A:155:LEU:HD22	1:B:190:ILE:HG23	1.99	0.44
1:A:130:GLU:O	1:A:132:ASP:N	2.47	0.44
1:A:177:LYS:NZ	1:A:179:ARG:NH2	2.64	0.44
1:B:35:ALA:C	1:B:37:TRP:N	2.70	0.44
1:A:12:ALA:HB1	1:A:21:LEU:HB2	1.98	0.44
1:A:31:GLN:C	1:A:33:LEU:H	2.21	0.44
1:A:168:ILE:C	1:A:168:ILE:HD12	2.38	0.44
1:B:225:TYR:N	1:B:225:TYR:HD1	2.13	0.44
1:A:227:PHE:CD1	1:A:230:LEU:CD1	3.00	0.44
1:B:151:VAL:HG13	1:B:189:LEU:HD22	2.00	0.43
1:A:36:LEU:O	1:A:37:TRP:C	2.57	0.43
1:A:98:GLN:HE21	1:A:127:ALA:CB	2.30	0.43
1:A:138:MSE:CE	1:A:211:THR:HG22	2.46	0.43
1:B:35:ALA:C	1:B:37:TRP:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:SER:HA	1:B:69:GLN:HE22	1.83	0.43
1:B:132:ASP:C	1:B:133:GLU:CG	2.86	0.43
1:A:28:ILE:HG23	1:A:28:ILE:O	2.17	0.43
1:A:146:ARG:HA	1:A:146:ARG:HD2	1.82	0.43
1:A:150:THR:C	1:A:152:GLU:N	2.69	0.43
1:B:37:TRP:HE1	1:B:45:ARG:NH1	2.16	0.43
1:B:177:LYS:NZ	1:B:179:ARG:NH2	2.66	0.43
1:A:35:ALA:C	1:A:37:TRP:N	2.72	0.43
1:A:169:TYR:HB3	1:A:170:TYR:CD1	2.53	0.43
1:A:215:GLN:NE2	1:A:251:VAL:HG11	2.33	0.43
1:B:5:LEU:HD13	1:B:27:GLU:O	2.19	0.43
1:B:69:GLN:O	1:B:73:LEU:HG	2.18	0.43
1:B:80:ARG:HD2	1:B:80:ARG:HA	1.81	0.43
1:B:208:TYR:CG	1:B:209:VAL:N	2.80	0.43
1:A:37:TRP:O	1:A:40:LEU:N	2.51	0.43
1:A:180:LEU:CD2	1:A:182:GLY:H	2.31	0.43
1:A:227:PHE:CD1	1:A:230:LEU:HD13	2.53	0.43
1:B:53:PRO:HG2	1:B:56:LYS:HD2	1.99	0.43
1:B:61:LEU:CD1	1:B:64:LEU:HD12	2.48	0.43
1:A:37:TRP:CE2	1:A:45:ARG:HG2	2.53	0.43
1:A:67:GLU:CD	1:A:67:GLU:N	2.71	0.43
1:B:169:TYR:HB3	1:B:170:TYR:CD1	2.54	0.43
1:B:169:TYR:HB3	1:B:170:TYR:CE1	2.53	0.43
1:A:5:LEU:HB3	1:A:24:VAL:CG1	2.49	0.43
1:A:162:ALA:N	1:A:163:PRO:HD2	2.31	0.43
1:B:5:LEU:CB	1:B:24:VAL:HG13	2.48	0.43
1:A:19:ARG:HD2	1:A:20:ALA:HB2	2.01	0.42
1:A:123:VAL:O	1:A:126:LEU:HB2	2.19	0.42
1:A:45:ARG:HB2	1:A:72:TYR:OH	2.19	0.42
1:A:187:ARG:NH2	1:B:167:THR:CA	2.79	0.42
1:A:7:VAL:HG22	1:A:10:GLN:HE22	1.78	0.42
1:B:36:LEU:O	1:B:37:TRP:C	2.56	0.42
1:A:19:ARG:CD	1:A:20:ALA:H	2.31	0.42
1:A:6:ALA:C	1:A:8:SER:N	2.71	0.42
1:A:90:LEU:O	1:A:93:LEU:HB2	2.20	0.42
1:A:139:THR:C	1:A:141:GLU:N	2.73	0.42
1:B:105:PRO:C	1:B:108:PHE:H	2.23	0.42
1:A:128:ARG:HH21	1:A:136:GLY:N	2.17	0.42
1:A:176:GLU:H	1:A:176:GLU:HG3	1.65	0.42
1:A:5:LEU:HD11	1:A:27:GLU:OE1	2.19	0.42
1:A:66:PRO:O	1:A:67:GLU:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:PRO:C	1:A:108:PHE:H	2.23	0.42
1:A:169:TYR:C	1:A:170:TYR:CD1	2.93	0.42
1:A:29:HIS:ND1	1:A:30:PRO:CD	2.81	0.42
1:A:154:VAL:O	1:A:155:LEU:C	2.58	0.42
1:A:207:VAL:HG11	1:A:225:TYR:HE2	1.75	0.42
1:B:132:ASP:O	1:B:133:GLU:HB3	2.19	0.42
1:A:33:LEU:C	1:A:35:ALA:N	2.73	0.42
1:A:70:ALA:HB2	1:A:100:VAL:HA	2.02	0.42
1:A:158:LEU:HA	1:A:158:LEU:HD12	1.84	0.42
1:A:190:ILE:HG23	1:B:155:LEU:CD2	2.47	0.42
1:B:21:LEU:O	1:B:25:LEU:HG	2.20	0.42
1:B:130:GLU:HB3	1:B:133:GLU:OE1	2.20	0.42
1:A:175:ASP:OD1	1:A:179:ARG:HG2	2.20	0.42
1:B:169:TYR:HD2	1:B:169:TYR:HA	1.79	0.42
1:B:222:MSE:CE	1:B:248:VAL:HG21	2.50	0.42
1:A:147:GLU:HB3	1:A:173:VAL:HG11	2.02	0.41
1:A:186:LEU:CD1	1:B:190:ILE:HD12	2.50	0.41
1:B:7:VAL:HG22	1:B:10:GLN:NE2	2.35	0.41
1:B:53:PRO:HG2	1:B:56:LYS:CD	2.50	0.41
1:A:35:ALA:C	1:A:37:TRP:H	2.23	0.41
1:A:101:ARG:HH22	1:A:129:TYR:H	1.67	0.41
1:B:33:LEU:C	1:B:35:ALA:N	2.72	0.41
1:B:219:ALA:HA	1:B:248:VAL:HG11	2.02	0.41
1:A:21:LEU:O	1:A:25:LEU:HG	2.19	0.41
1:A:128:ARG:CZ	1:A:135:GLY:O	2.67	0.41
1:B:10:GLN:O	1:B:14:GLN:NE2	2.53	0.41
1:B:11:GLU:C	1:B:13:LEU:N	2.73	0.41
1:B:154:VAL:O	1:B:155:LEU:C	2.59	0.41
1:A:205:LYS:HE3	1:A:205:LYS:HB2	1.87	0.41
1:B:37:TRP:O	1:B:40:LEU:N	2.50	0.41
1:B:132:ASP:C	1:B:133:GLU:HG2	2.41	0.41
1:B:142:TYR:CB	1:B:242:ILE:HG21	2.48	0.41
1:A:5:LEU:CA	1:A:8:SER:HB3	2.50	0.41
1:A:90:LEU:O	1:A:93:LEU:HB3	2.21	0.41
1:B:180:LEU:CD2	1:B:180:LEU:C	2.89	0.41
1:A:91:ASP:C	1:A:93:LEU:H	2.24	0.41
1:A:142:TYR:CB	1:A:242:ILE:HG21	2.44	0.41
1:A:208:TYR:HD2	1:A:209:VAL:H	1.68	0.41
1:B:28:ILE:HD12	1:B:28:ILE:HA	1.93	0.41
1:B:47:VAL:O	1:B:47:VAL:HG12	2.21	0.41
1:A:88:LEU:CD2	1:A:93:LEU:HA	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ILE:CD1	1:A:186:LEU:HD22	2.51	0.41
1:A:207:VAL:HG23	1:A:230:LEU:HD11	2.03	0.41
1:B:5:LEU:HB3	1:B:28:ILE:HD13	2.03	0.41
1:B:37:TRP:C	1:B:39:GLU:N	2.74	0.41
1:B:127:ALA:O	1:B:128:ARG:HB3	2.20	0.41
1:B:179:ARG:HB2	1:B:237:GLY:O	2.21	0.41
1:B:66:PRO:O	1:B:67:GLU:C	2.59	0.41
1:B:129:TYR:N	1:B:129:TYR:CD2	2.89	0.41
1:A:80:ARG:HD2	1:A:80:ARG:HA	1.83	0.40
1:B:218:VAL:O	1:B:218:VAL:CG1	2.69	0.40
1:B:218:VAL:O	1:B:222:MSE:CB	2.69	0.40
1:A:11:GLU:C	1:A:13:LEU:N	2.75	0.40
1:A:66:PRO:HG2	1:A:67:GLU:H	1.87	0.40
1:B:90:LEU:O	1:B:94:ALA:N	2.54	0.40
1:B:94:ALA:O	1:B:98:GLN:HG3	2.21	0.40
1:B:203:ASN:OD1	1:B:205:LYS:N	2.40	0.40
1:A:159:ARG:HG2	1:B:191:VAL:HA	2.03	0.40
1:B:94:ALA:HB2	1:B:126:LEU:CD2	2.47	0.40
1:B:218:VAL:O	1:B:222:MSE:HB3	2.21	0.40
1:A:56:LYS:O	1:A:57:ALA:C	2.60	0.40
1:B:208:TYR:O	1:B:209:VAL:HB	2.21	0.40
1:B:90:LEU:O	1:B:93:LEU:CB	2.68	0.40
1:B:101:ARG:NH1	1:B:128:ARG:HA	2.37	0.40
1:B:172:TYR:CE2	1:B:231:PRO:CB	2.99	0.40
1:B:207:VAL:CG2	1:B:227:PHE:CE1	3.00	0.40
1:B:218:VAL:HG12	1:B:222:MSE:HE2	2.02	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	246/278 (88%)	182 (74%)	43 (18%)	21 (8%)	1 13
1	B	246/278 (88%)	185 (75%)	41 (17%)	20 (8%)	1 14
All	All	492/556 (88%)	367 (75%)	84 (17%)	41 (8%)	1 14

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	TRP
1	A	38	ASP
1	A	54	LYS
1	A	102	LYS
1	A	127	ALA
1	A	131	GLU
1	A	132	ASP
1	A	134	ALA
1	A	200	GLU
1	B	37	TRP
1	B	38	ASP
1	B	54	LYS
1	B	127	ALA
1	B	133	GLU
1	B	200	GLU
1	A	6	ALA
1	A	14	GLN
1	A	69	GLN
1	A	140	PRO
1	A	209	VAL
1	B	6	ALA
1	B	14	GLN
1	B	69	GLN
1	B	102	LYS
1	B	128	ARG
1	B	140	PRO
1	A	32	ASP
1	A	34	LEU
1	A	40	LEU
1	A	128	ARG
1	B	32	ASP
1	B	34	LEU
1	B	40	LEU
1	B	209	VAL
1	A	10	GLN

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Mol	Chain	Res	Type
1	B	10	GLN
1	B	96	ALA
1	A	66	PRO
1	A	96	ALA
1	B	66	PRO
1	B	131	GLU

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	215/235 (92%)	199 (93%)	16 (7%)	13	43
1	B	215/235 (92%)	200 (93%)	15 (7%)	15	44
All	All	430/470 (92%)	399 (93%)	31 (7%)	14	44

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	31	GLN
1	A	33	LEU
1	A	36	LEU
1	A	89	SER
1	A	93	LEU
1	A	95	ASP
1	A	103	GLU
1	A	117	PRO
1	A	128	ARG
1	A	129	TYR
1	A	139	THR
1	A	146	ARG
1	A	196	THR
1	A	250	ASP
1	A	252	LEU
1	B	19	ARG

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Mol	Chain	Res	Type
1	B	30	PRO
1	B	31	GLN
1	B	33	LEU
1	B	36	LEU
1	B	48	VAL
1	B	93	LEU
1	B	128	ARG
1	B	146	ARG
1	B	168	ILE
1	B	169	TYR
1	B	180	LEU
1	B	196	THR
1	B	216	GLU
1	B	252	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	215	GLN
1	B	10	GLN
1	B	215	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 (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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	244/278 (87%)	0.28	25 (10%)	6	6	161, 228, 266, 287	0
1	B	244/278 (87%)	0.68	49 (20%)	1	1	162, 225, 261, 277	0
All	All	488/556 (87%)	0.48	74 (15%)	2	2	161, 226, 265, 287	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	TYR	8.5
1	B	231	PRO	8.5
1	B	230	LEU	8.4
1	B	50	THR	7.0
1	B	72	TYR	6.6
1	B	63	HIS	6.1
1	A	73	LEU	5.8
1	B	242	ILE	5.8
1	B	241	GLY	5.8
1	B	168	ILE	5.1
1	A	70	ALA	4.9
1	B	172	TYR	4.7
1	B	131	GLU	4.2
1	B	73	LEU	4.1
1	B	144	ALA	4.1
1	B	74	LYS	4.1
1	A	168	ILE	3.9
1	B	243	VAL	3.9
1	A	44	HIS	3.9
1	A	225	TYR	3.8
1	A	49	LEU	3.7
1	B	252	LEU	3.6
1	B	229	VAL	3.5
1	B	44	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	47	VAL	3.4
1	A	46	TYR	3.3
1	B	164	ASP	3.3
1	A	50	THR	3.3
1	A	107	TYR	3.2
1	B	85	LEU	3.1
1	B	145	VAL	3.0
1	A	69	GLN	3.0
1	B	34	LEU	2.8
1	B	177	LYS	2.8
1	B	158	LEU	2.8
1	B	61	LEU	2.8
1	A	76	LEU	2.8
1	B	232	VAL	2.7
1	B	37	TRP	2.7
1	A	101	ARG	2.7
1	B	165	ALA	2.7
1	B	51	LEU	2.6
1	A	166	GLU	2.6
1	B	76	LEU	2.6
1	B	129	TYR	2.6
1	A	75	THR	2.6
1	A	52	LEU	2.6
1	A	169	TYR	2.6
1	B	33	LEU	2.5
1	B	54	LYS	2.5
1	B	46	TYR	2.5
1	B	240	VAL	2.5
1	B	215	GLN	2.5
1	A	11	GLU	2.5
1	B	103	GLU	2.4
1	B	59	GLU	2.4
1	B	69	GLN	2.3
1	B	251	VAL	2.3
1	A	84	ILE	2.3
1	B	48	VAL	2.2
1	A	111	LEU	2.2
1	A	186	LEU	2.2
1	A	229	VAL	2.2
1	B	189	LEU	2.2
1	A	183	VAL	2.1
1	A	228	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	80	ARG	2.1
1	B	40	LEU	2.1
1	B	111	LEU	2.1
1	B	126	LEU	2.0
1	B	170	TYR	2.0
1	B	207	VAL	2.0
1	B	32	ASP	2.0
1	B	239	LEU	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.