Full wwPDB X-ray Structure Validation Report (i)

Jul 27, 2016 – 03:51 PM EDT

PDB ID	:	5ITR
Title	:	Crystal Structure of Human NEIL1(P2G) bound to duplex DNA containing THF
Authors	:	Zhu, C.; Lu, L.; Zhang, J.; Yue, Z.; Song, J.; Zong, S.; Liu, M.; Stovicek, O.; Gao, Y.; Yi, C.
Deposited on	:	2016-03-17
Resolution	:	2.46 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

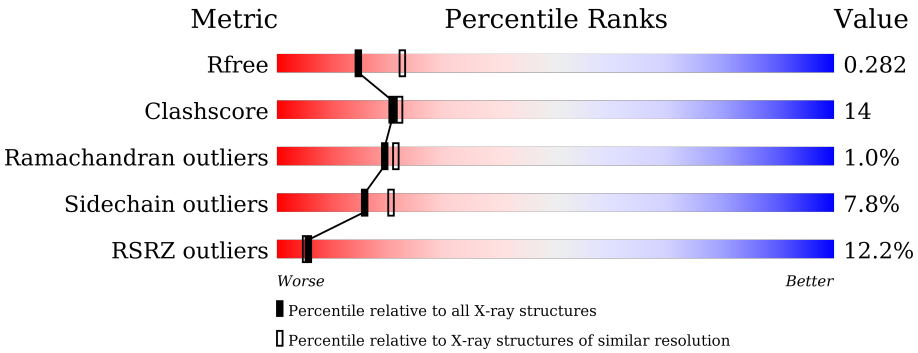
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.46 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	400	3% 52% 12% · 33%
1	B	400	3% 46% 16% · 35%
1	C	400	19% 44% 18% · 37%
2	D	26	8% 77% 23%
2	E	26	65% 31% ·
3	F	26	12% 54% 46%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7925 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 Endonuclease 8-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	2	0
			2146	1369	393	374	10			
1	B	261	Total	C	N	O	S	0	0	0
			2073	1324	381	358	10			
1	C	254	Total	C	N	O	S	0	0	0
			2032	1302	371	349	10			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	ARG	LYS	engineered mutation	UNP Q96FI4
A	391	ALA	-	expression tag	UNP Q96FI4
A	392	ALA	-	expression tag	UNP Q96FI4
A	393	LEU	-	expression tag	UNP Q96FI4
A	394	GLY	-	expression tag	UNP Q96FI4
A	395	HIS	-	expression tag	UNP Q96FI4
A	396	HIS	-	expression tag	UNP Q96FI4
A	397	HIS	-	expression tag	UNP Q96FI4
A	398	HIS	-	expression tag	UNP Q96FI4
A	399	HIS	-	expression tag	UNP Q96FI4
A	400	HIS	-	expression tag	UNP Q96FI4
B	242	ARG	LYS	engineered mutation	UNP Q96FI4
B	391	ALA	-	expression tag	UNP Q96FI4
B	392	ALA	-	expression tag	UNP Q96FI4
B	393	LEU	-	expression tag	UNP Q96FI4
B	394	GLY	-	expression tag	UNP Q96FI4
B	395	HIS	-	expression tag	UNP Q96FI4
B	396	HIS	-	expression tag	UNP Q96FI4
B	397	HIS	-	expression tag	UNP Q96FI4
B	398	HIS	-	expression tag	UNP Q96FI4
B	399	HIS	-	expression tag	UNP Q96FI4
B	400	HIS	-	expression tag	UNP Q96FI4
C	242	ARG	LYS	engineered mutation	UNP Q96FI4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	391	ALA	-	expression tag	UNP Q96FI4
C	392	ALA	-	expression tag	UNP Q96FI4
C	393	LEU	-	expression tag	UNP Q96FI4
C	394	GLY	-	expression tag	UNP Q96FI4
C	395	HIS	-	expression tag	UNP Q96FI4
C	396	HIS	-	expression tag	UNP Q96FI4
C	397	HIS	-	expression tag	UNP Q96FI4
C	398	HIS	-	expression tag	UNP Q96FI4
C	399	HIS	-	expression tag	UNP Q96FI4
C	400	HIS	-	expression tag	UNP Q96FI4

- Molecule 2 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	26	Total	C	N	O	P	0	0	0
			516	247	94	151	24			
2	E	26	Total	C	N	O	P	0	0	0
			516	247	94	151	24			

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	26	Total	C	N	O	P	0	0	0
			517	247	94	152	24			

- Molecule 4 is water.

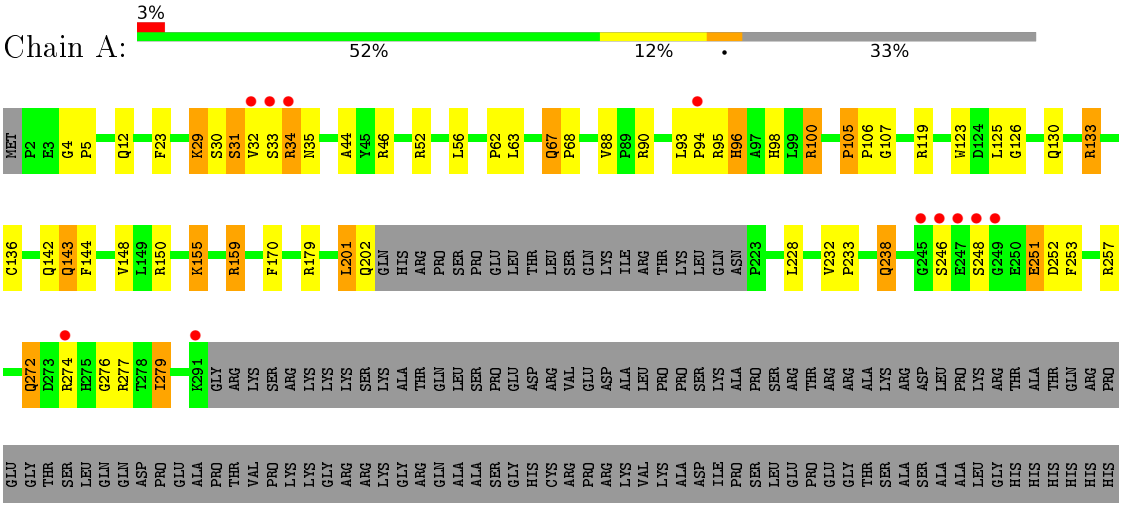
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	B	45	Total	O	0	0
			45	45		
4	C	4	Total	O	0	0
			4	4		
4	D	9	Total	O	0	0
			9	9		
4	E	8	Total	O	0	0
			8	8		

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

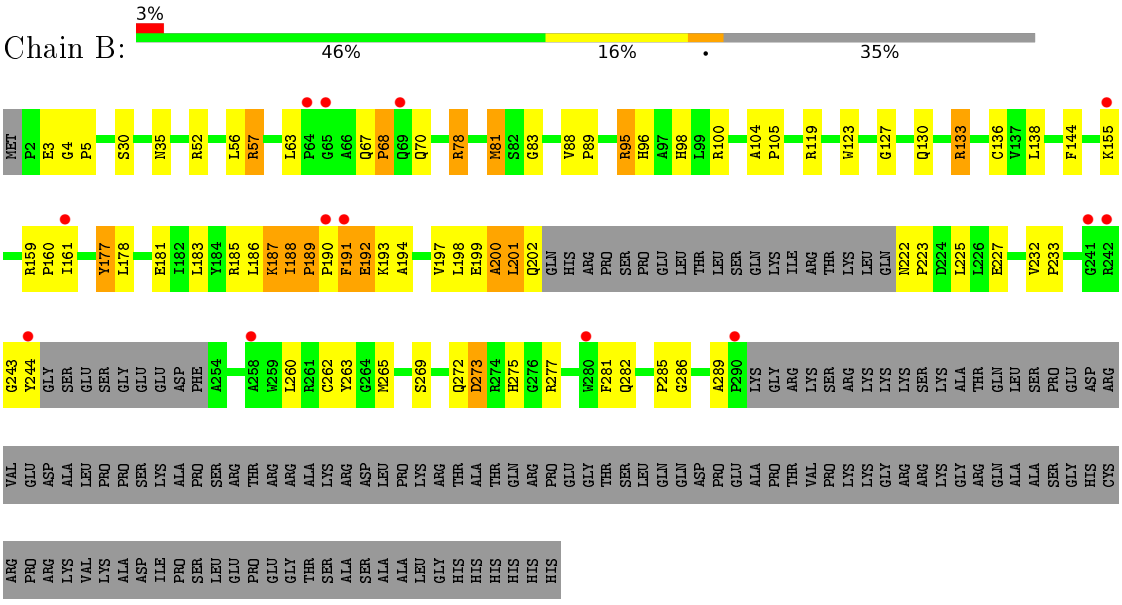
- Molecule 1: Endonuclease 8-like 1

Chain A:



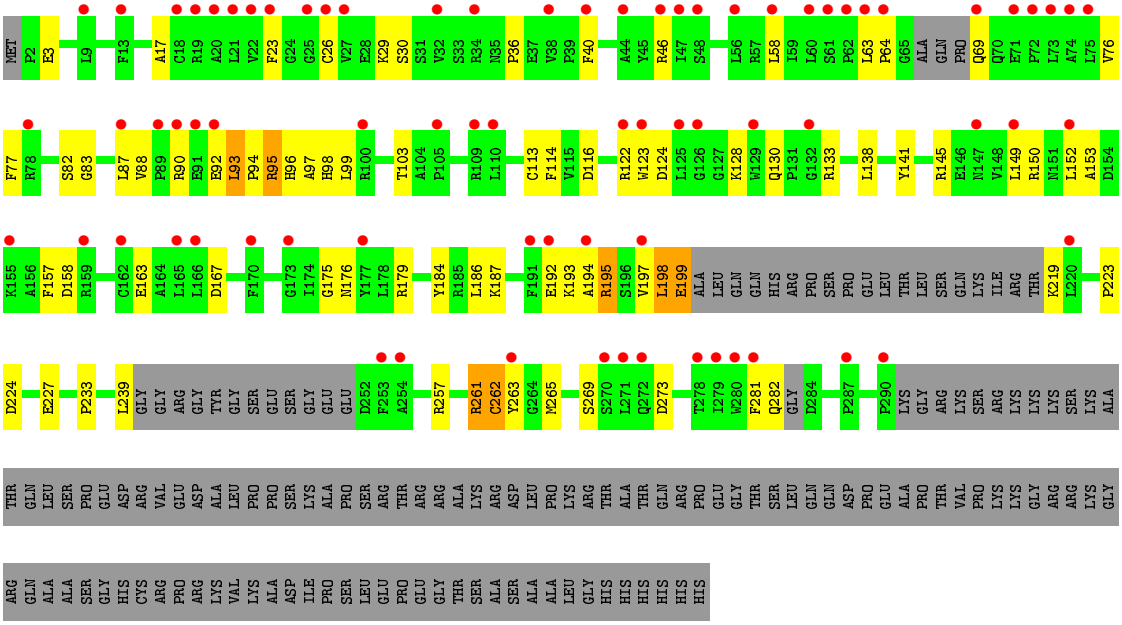
- Molecule 1: Endonuclease 8-like 1

Chain B:

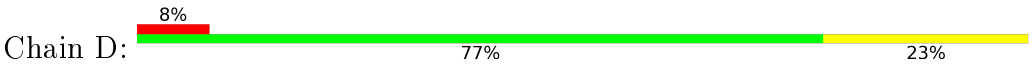


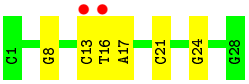
- Molecule 1: Endonuclease 8-like 1

Chain C:

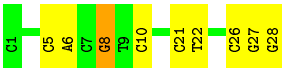


- Molecule 2: DNA (26-MER)

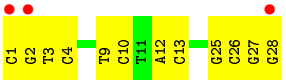




- Molecule 2: DNA (26-MER)



- Molecule 3: DNA (26-MER)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.31Å 109.04Å 169.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.75 – 2.46 44.81 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.4 (91.75-2.46) 99.4 (44.81-2.46)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.211 , 0.263 0.240 , 0.282	Depositor DCC
R_{free} test set	2484 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7925	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.01	0/2211	1.01	8/2989 (0.3%)
1	B	0.94	2/2129 (0.1%)	1.01	10/2879 (0.3%)
1	C	0.49	0/2085	0.70	1/2816 (0.0%)
2	D	0.53	1/577 (0.2%)	0.83	0/886
2	E	0.56	1/577 (0.2%)	0.97	2/886 (0.2%)
3	F	0.41	0/578	0.76	0/888
All	All	0.79	4/8157 (0.0%)	0.91	21/11344 (0.2%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	21	DC	O3'-P	-5.36	1.54	1.61
2	E	8	DG	O3'-P	5.11	1.67	1.61
1	B	83	GLY	C-O	-5.11	1.15	1.23
1	B	189	PRO	N-CD	5.08	1.54	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	133	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	B	57	ARG	NE-CZ-NH2	-8.81	115.90	120.30
2	E	8	DG	O5'-P-OP1	-8.30	98.23	105.70
1	A	133	ARG	NE-CZ-NH2	-8.15	116.22	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	179	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	B	133	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	133	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	119	ARG	NE-CZ-NH2	-6.59	117.00	120.30
2	E	8	DG	O5'-P-OP2	6.51	118.52	110.70
1	A	179	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	68	PRO	N-CA-C	-5.94	96.65	112.10
1	C	93	LEU	C-N-CD	5.88	140.75	128.40
1	B	57	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	119	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	265	MET	C-N-CD	5.82	140.62	128.40
1	B	78	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	188	ILE	C-N-CD	5.60	140.16	128.40
1	B	78	ARG	CG-CD-NE	-5.30	100.68	111.80
1	A	126	GLY	N-CA-C	-5.18	100.15	113.10
1	A	67	GLN	C-N-CD	-5.16	109.25	120.60
1	A	119	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67	GLN	Mainchain,Peptide
1	B	67	GLN	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	2146	0	2109	81	0
1	B	2073	0	2055	66	0
1	C	2032	0	2016	53	0
2	D	516	0	290	5	0
2	E	516	0	290	6	0
3	F	517	0	290	10	0
4	A	59	0	0	1	2
4	B	45	0	0	1	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	4	0	0	0	0
4	D	9	0	0	1	0
4	E	8	0	0	1	0
All	All	7925	0	7050	215	2

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 14.

All (215) 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:191:PHE:CE2	1:B:289:ALA:HB2	1.16	1.58
1:B:191:PHE:CE2	1:B:289:ALA:CB	1.97	1.47
1:B:191:PHE:CZ	1:B:289:ALA:CB	2.10	1.32
1:B:191:PHE:CZ	1:B:289:ALA:HB2	1.75	1.16
1:B:191:PHE:CD2	1:B:289:ALA:HB2	1.81	1.15
1:B:191:PHE:CE1	1:B:289:ALA:HA	1.82	1.13
1:C:193:LYS:HD3	1:C:195:ARG:HB2	1.29	1.10
1:A:29:LYS:HZ3	1:A:33:SER:HB3	0.93	1.10
1:A:29:LYS:NZ	1:A:33:SER:HB3	1.67	1.07
1:B:191:PHE:CZ	1:B:289:ALA:CA	2.43	1.01
1:B:191:PHE:CZ	1:B:289:ALA:HA	1.97	1.00
1:B:191:PHE:HB2	1:B:285:PRO:O	1.63	0.99
1:A:30:SER:OG	1:A:98:HIS:HA	1.61	0.99
1:C:158:ASP:OD1	1:C:195:ARG:NH1	1.96	0.99
1:A:95:ARG:CD	1:A:96:HIS:HA	1.93	0.98
1:C:198:LEU:HD12	1:C:198:LEU:H	1.28	0.96
1:A:257[B]:ARG:HH21	1:A:257[B]:ARG:HG3	1.34	0.93
1:C:193:LYS:HD3	1:C:195:ARG:CB	1.98	0.93
1:A:30:SER:HB3	1:A:100:ARG:NH1	1.84	0.93
1:A:95:ARG:HE	1:A:96:HIS:HB3	1.35	0.91
1:A:29:LYS:HZ3	1:A:33:SER:CB	1.81	0.91
1:B:191:PHE:CZ	1:B:289:ALA:HB1	2.05	0.87
1:C:193:LYS:CD	1:C:195:ARG:HB2	2.06	0.85
1:B:191:PHE:CE1	1:B:289:ALA:CA	2.59	0.85
1:C:198:LEU:O	1:C:199:GLU:HG3	1.81	0.81
1:A:95:ARG:CG	1:A:96:HIS:HA	2.11	0.80
1:A:257[B]:ARG:HH21	1:A:257[B]:ARG:CG	1.94	0.80
1:A:201:LEU:O	1:A:202:GLN:HB2	1.83	0.78
1:C:198:LEU:O	1:C:199:GLU:CG	2.32	0.77
1:A:95:ARG:HD2	1:A:96:HIS:HA	1.63	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:PHE:CD2	1:B:285:PRO:HB2	2.20	0.77
1:A:29:LYS:CE	1:A:33:SER:HB3	2.14	0.75
1:B:260:LEU:HD22	1:B:263:TYR:HB3	1.68	0.75
1:B:191:PHE:HD2	1:B:285:PRO:HB2	1.51	0.74
1:B:191:PHE:HB3	1:B:286:GLY:C	2.07	0.74
1:B:189:PRO:HD2	1:B:192:GLU:OE2	1.89	0.73
1:A:34:ARG:HH11	1:A:34:ARG:HG2	1.53	0.73
1:B:191:PHE:CE2	1:B:289:ALA:HB1	2.13	0.71
2:D:24:DG:N7	4:D:101:HOH:O	2.24	0.70
1:A:105:PRO:O	1:A:107:GLY:N	2.25	0.69
1:A:246:SER:HB2	1:A:252:ASP:OD1	1.92	0.69
1:B:78:ARG:NH1	2:E:10:DC:OP2	2.26	0.69
1:A:277:ARG:NH2	2:D:8:DG:OP2	2.26	0.67
1:A:30:SER:O	1:A:33:SER:HB2	1.96	0.66
1:A:96:HIS:HB2	1:A:98:HIS:NE2	2.11	0.65
1:A:29:LYS:HE2	1:A:33:SER:O	1.96	0.65
1:B:273:ASP:OD2	1:B:277:ARG:HB2	1.97	0.65
1:C:198:LEU:HD12	1:C:198:LEU:N	2.02	0.65
1:A:246:SER:CB	1:A:252:ASP:OD1	2.45	0.64
1:B:104:ALA:HB1	1:B:105:PRO:HD2	1.80	0.64
1:C:198:LEU:C	1:C:199:GLU:CG	2.65	0.64
3:F:27:DG:H2'	3:F:28:DG:C8	2.31	0.64
1:A:202:GLN:HG2	1:A:202:GLN:O	1.98	0.63
1:B:193:LYS:O	1:B:197:VAL:HG23	1.99	0.62
1:A:88:VAL:HG21	1:A:94:PRO:CD	2.29	0.62
1:A:34:ARG:HG2	1:A:34:ARG:NH1	2.14	0.62
1:B:191:PHE:HB2	1:B:285:PRO:C	2.21	0.61
1:B:191:PHE:HB2	1:B:286:GLY:CA	2.30	0.61
1:C:197:VAL:HG13	1:C:197:VAL:O	2.01	0.60
1:B:30:SER:HB3	1:B:98:HIS:HA	1.83	0.60
1:A:88:VAL:HG21	1:A:94:PRO:HD3	1.84	0.60
1:B:191:PHE:HB2	1:B:286:GLY:HA3	1.83	0.60
1:C:153:ALA:O	1:C:195:ARG:NH2	2.35	0.60
1:A:30:SER:HG	1:A:98:HIS:HA	1.66	0.60
1:A:29:LYS:HD2	1:A:33:SER:OG	2.02	0.59
1:C:176:ASN:O	1:C:179:ARG:HG2	2.02	0.59
1:A:95:ARG:HG3	1:A:96:HIS:HA	1.85	0.58
1:B:222:ASN:N	1:B:223:PRO:CD	2.66	0.58
1:A:29:LYS:CG	1:A:33:SER:CB	2.82	0.58
1:A:95:ARG:HE	1:A:96:HIS:CB	2.14	0.58
1:A:96:HIS:O	1:A:98:HIS:CD2	2.57	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LEU:HB2	1:B:188:ILE:HD12	1.84	0.58
1:A:257[B]:ARG:NH2	1:A:257[B]:ARG:CG	2.58	0.57
1:C:152:LEU:O	1:C:195:ARG:NH2	2.36	0.56
1:C:193:LYS:HE2	1:C:195:ARG:HD2	1.88	0.56
1:A:96:HIS:CD2	1:A:96:HIS:N	2.73	0.56
1:A:31:SER:O	1:A:32:VAL:HG12	2.06	0.55
1:A:46:ARG:HG3	1:A:63:LEU:HD21	1.87	0.55
1:A:90:ARG:O	1:A:93:LEU:CD1	2.54	0.55
1:C:193:LYS:HG2	1:C:195:ARG:H	1.71	0.55
1:C:198:LEU:O	1:C:199:GLU:CB	2.53	0.55
1:C:23:PHE:HA	1:C:103:THR:HA	1.88	0.55
2:E:28:DG:OP1	2:E:28:DG:H4'	2.07	0.55
2:D:13:DC:H2"	3:F:1:DC:C6	2.41	0.55
1:B:200:ALA:O	1:B:201:LEU:HD12	2.07	0.55
1:A:277:ARG:HH22	2:D:8:DG:P	2.30	0.54
1:A:29:LYS:CD	1:A:33:SER:HB3	2.37	0.54
1:A:90:ARG:O	1:A:93:LEU:HD13	2.07	0.54
1:C:99:LEU:HD22	1:C:123:TRP:CE2	2.42	0.54
3:F:3:DT:H3	3:F:25:DG:H1	1.55	0.54
1:A:159:ARG:NH2	1:A:274:ARG:HE	2.06	0.54
1:A:30:SER:HB3	1:A:100:ARG:HH12	1.69	0.53
1:A:130:GLN:NE2	1:A:133:ARG:HD2	2.24	0.53
1:C:138:LEU:HD21	1:C:233:PRO:HB2	1.91	0.53
1:B:191:PHE:CB	1:B:286:GLY:C	2.77	0.52
1:C:198:LEU:C	1:C:199:GLU:HG2	2.30	0.52
1:B:198:LEU:HD21	1:B:225:LEU:HD23	1.90	0.52
1:C:29:LYS:NZ	1:C:30:SER:O	2.39	0.52
1:A:88:VAL:HG11	1:A:94:PRO:HG3	1.92	0.51
1:C:263:TYR:O	1:C:265:MET:HG2	2.10	0.51
3:F:9:DT:H2"	3:F:10:DC:OP1	2.10	0.51
1:A:95:ARG:HG3	1:A:96:HIS:CA	2.40	0.51
3:F:25:DG:H2"	3:F:26:DC:OP2	2.10	0.51
1:B:223:PRO:HA	1:B:227:GLU:OE2	2.09	0.51
1:A:29:LYS:CG	1:A:33:SER:HB3	2.41	0.51
1:B:191:PHE:CB	1:B:286:GLY:CA	2.89	0.51
1:B:199:GLU:O	1:B:202:GLN:HG2	2.11	0.50
1:B:222:ASN:N	1:B:223:PRO:HD2	2.26	0.50
1:A:201:LEU:O	1:A:202:GLN:CB	2.54	0.50
1:A:88:VAL:HG21	1:A:94:PRO:HD2	1.94	0.50
1:A:96:HIS:HB2	1:A:98:HIS:CE1	2.46	0.50
1:B:159:ARG:HB3	1:B:160:PRO:HD2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:HG2	1:A:33:SER:HB3	1.94	0.49
1:C:157:PHE:HA	1:C:194:ALA:HB3	1.93	0.49
1:A:150:ARG:HG2	1:A:150:ARG:O	2.13	0.49
1:A:257[B]:ARG:NH2	4:A:505:HOH:O	2.45	0.48
1:B:198:LEU:O	1:B:201:LEU:HD12	2.13	0.48
1:C:223:PRO:HA	1:C:227:GLU:OE1	2.13	0.48
1:B:138:LEU:HD21	1:B:233:PRO:HB2	1.95	0.48
1:B:191:PHE:CB	1:B:286:GLY:HA3	2.42	0.48
1:A:30:SER:HB3	1:A:100:ARG:HH11	1.72	0.48
3:F:2:DG:H2"	3:F:3:DT:O5'	2.13	0.48
1:C:163:GLU:CG	1:C:273:ASP:HB2	2.44	0.48
1:A:4:GLY:N	1:A:5:PRO:CD	2.77	0.48
1:A:95:ARG:NE	1:A:96:HIS:HA	2.27	0.48
1:C:157:PHE:O	1:C:194:ALA:HB3	2.13	0.47
1:C:193:LYS:HG2	1:C:194:ALA:N	2.28	0.47
1:A:29:LYS:HG2	1:A:33:SER:CB	2.44	0.47
1:B:4:GLY:N	1:B:5:PRO:CD	2.77	0.47
1:C:193:LYS:NZ	1:C:195:ARG:HD3	2.29	0.47
1:C:90:ARG:O	1:C:93:LEU:HD11	2.14	0.47
1:A:279:ILE:HG23	1:A:279:ILE:O	2.14	0.47
1:A:155:LYS:HE3	1:A:155:LYS:N	2.30	0.47
1:B:188:ILE:O	1:B:190:PRO:HD3	2.15	0.47
1:B:198:LEU:CD2	1:B:225:LEU:HD23	2.45	0.47
1:A:32:VAL:HG22	1:A:32:VAL:O	2.15	0.47
1:C:58:LEU:HD12	1:C:77:PHE:HE1	1.79	0.47
1:B:189:PRO:HB2	1:B:192:GLU:HG2	1.97	0.46
1:C:130:GLN:HB3	1:C:133:ARG:HD2	1.96	0.46
1:C:193:LYS:CE	1:C:195:ARG:HB2	2.45	0.46
1:A:56:LEU:C	1:A:56:LEU:HD23	2.36	0.46
1:A:96:HIS:H	1:A:96:HIS:CD2	2.32	0.46
1:B:88:VAL:HB	1:B:89:PRO:HD2	1.96	0.46
1:C:184:TYR:CE2	1:C:261:ARG:O	2.69	0.46
1:C:262:CYS:O	1:C:265:MET:HB2	2.15	0.46
1:C:157:PHE:CA	1:C:194:ALA:HB3	2.44	0.46
2:D:16:DT:H4'	2:D:17:DA:OP1	2.15	0.46
1:C:149:LEU:O	1:C:152:LEU:HG	2.15	0.46
1:B:57:ARG:NH1	1:B:127:GLY:O	2.42	0.46
1:B:243:GLY:O	1:B:244:TYR:HB2	2.15	0.46
1:A:29:LYS:CD	1:A:33:SER:CB	2.93	0.46
1:A:52:ARG:HG3	1:A:136:CYS:HB2	1.97	0.46
1:C:198:LEU:HD13	1:C:198:LEU:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:CYS:HA	1:C:40:PHE:O	2.15	0.45
3:F:12:DA:H1'	3:F:13:DC:O5'	2.16	0.45
1:C:17:ALA:HB1	1:C:87:LEU:HD22	1.97	0.45
3:F:27:DG:C6	3:F:28:DG:O6	2.69	0.45
1:C:58:LEU:HD12	1:C:77:PHE:CE1	2.50	0.45
1:A:155:LYS:HD3	3:F:27:DG:OP1	2.16	0.45
1:A:35:ASN:HB3	1:A:123:TRP:CE2	2.51	0.45
1:B:232:VAL:HB	1:B:233:PRO:CD	2.46	0.45
1:B:181:GLU:O	1:B:185:ARG:HG3	2.16	0.45
2:E:21:DC:H2'	2:E:22:DT:C6	2.52	0.45
1:A:272:GLN:NE2	1:A:276:GLY:O	2.50	0.45
1:B:81:MET:SD	2:E:8:DG:H5"	2.57	0.45
1:B:130:GLN:HB3	1:B:133:ARG:CD	2.47	0.44
1:C:96:HIS:O	1:C:98:HIS:CD2	2.70	0.44
1:B:35:ASN:HB2	1:B:123:TRP:CZ2	2.53	0.44
1:B:56:LEU:C	1:B:56:LEU:HD23	2.37	0.44
1:A:29:LYS:CD	1:A:33:SER:OG	2.65	0.44
1:A:253:PHE:CZ	1:A:257[B]:ARG:HD2	2.52	0.44
1:B:198:LEU:HA	1:B:201:LEU:CD1	2.47	0.44
1:C:141:TYR:OH	1:C:145:ARG:NH1	2.44	0.44
1:C:114:PHE:CE2	1:C:116:ASP:HB2	2.53	0.43
1:B:189:PRO:CD	1:B:192:GLU:OE2	2.63	0.43
2:E:5:DC:H2"	2:E:6:DA:C8	2.53	0.43
1:B:273:ASP:OD1	1:B:275:HIS:N	2.50	0.43
1:B:70:GLN:NE2	4:B:503:HOH:O	2.52	0.43
1:B:183:LEU:O	1:B:187:LYS:N	2.52	0.43
1:C:269:SER:HB3	1:C:281:PHE:CZ	2.54	0.42
1:A:142:GLN:CD	1:A:142:GLN:H	2.22	0.42
1:C:186:LEU:O	1:C:187:LYS:C	2.58	0.42
1:A:23:PHE:O	1:A:44:ALA:HA	2.19	0.42
1:C:88:VAL:HG21	1:C:94:PRO:HD3	2.01	0.42
1:A:143:GLN:H	1:A:143:GLN:HE21	1.67	0.42
1:C:82:SER:O	1:C:83:GLY:C	2.57	0.42
1:A:96:HIS:CB	1:A:98:HIS:CE1	3.03	0.42
1:B:3:GLU:OE2	1:B:177:TYR:CD2	2.72	0.42
1:B:81:MET:HE1	4:E:104:HOH:O	2.20	0.42
1:C:3:GLU:OE1	1:C:175:GLY:N	2.53	0.42
1:C:63:LEU:HD22	1:C:64:PRO:HD2	2.02	0.42
1:A:246:SER:HB3	1:A:252:ASP:OD1	2.18	0.42
1:A:30:SER:OG	1:A:98:HIS:CA	2.50	0.42
1:A:232:VAL:HB	1:A:233:PRO:CD	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ARG:HB3	1:C:96:HIS:CD2	2.54	0.42
1:B:262:CYS:SG	1:B:281:PHE:HA	2.60	0.42
1:A:148:VAL:HG22	1:A:170:PHE:HB3	2.02	0.41
3:F:3:DT:H2'	3:F:4:DC:C6	2.55	0.41
1:A:228:LEU:O	1:A:232:VAL:HG23	2.20	0.41
1:C:224:ASP:OD1	1:C:224:ASP:C	2.59	0.41
1:A:29:LYS:HE2	1:A:35:ASN:O	2.20	0.41
1:A:32:VAL:HG13	1:A:32:VAL:O	2.21	0.41
2:E:26:DC:H2"	2:E:27:DG:C8	2.56	0.41
1:B:189:PRO:HB2	1:B:192:GLU:CG	2.51	0.40
1:B:52:ARG:HG3	1:B:136:CYS:HB2	2.02	0.40
1:B:95:ARG:HG3	1:B:96:HIS:CD2	2.56	0.40
1:A:238:GLN:HE21	1:A:238:GLN:HB3	1.66	0.40
1:B:161:ILE:HA	1:B:194:ALA:HB2	2.03	0.40
1:B:178:LEU:HD23	1:B:178:LEU:HA	1.94	0.40
1:B:130:GLN:NE2	1:B:133:ARG:HH11	2.18	0.40
1:C:76:VAL:HG21	1:C:128:LYS:O	2.21	0.40
1:A:95:ARG:HG3	1:A:96:HIS:CG	2.56	0.40
1:B:130:GLN:HB3	1:B:133:ARG:HD2	2.02	0.40
1:A:251:GLU:H	1:A:251:GLU:HG3	1.53	0.40
1:C:269:SER:HB3	1:C:281:PHE:CE1	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:551:HOH:O	4:B:525:HOH:O[3_555]	1.81	0.39
4:A:558:HOH:O	4:B:537:HOH:O[3_555]	1.99	0.21

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	268/400 (67%)	251 (94%)	15 (6%)	2 (1%)	26 32
1	B	255/400 (64%)	231 (91%)	22 (9%)	2 (1%)	24 28
1	C	244/400 (61%)	215 (88%)	25 (10%)	4 (2%)	12 11
All	All	767/1200 (64%)	697 (91%)	62 (8%)	8 (1%)	19 21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	PRO
1	B	68	PRO
1	B	200	ALA
1	C	36	PRO
1	C	97	ALA
1	C	262	CYS
1	C	167	ASP
1	A	106	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	222/335 (66%)	203 (91%)	19 (9%)	13 16
1	B	216/335 (64%)	201 (93%)	15 (7%)	19 25
1	C	214/335 (64%)	197 (92%)	17 (8%)	15 20
All	All	652/1005 (65%)	601 (92%)	51 (8%)	16 20

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	29	LYS
1	A	31	SER
1	A	34	ARG
1	A	62	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	96	HIS
1	A	100	ARG
1	A	105	PRO
1	A	125	LEU
1	A	143	GLN
1	A	144	PHE
1	A	155	LYS
1	A	159	ARG
1	A	201	LEU
1	A	238	GLN
1	A	248	SER
1	A	251	GLU
1	A	272	GLN
1	A	279	ILE
1	B	63	LEU
1	B	81	MET
1	B	95	ARG
1	B	100	ARG
1	B	144	PHE
1	B	155	LYS
1	B	177	TYR
1	B	187	LYS
1	B	191	PHE
1	B	192	GLU
1	B	201	LEU
1	B	269	SER
1	B	272	GLN
1	B	273	ASP
1	B	282	GLN
1	C	46	ARG
1	C	69	GLN
1	C	92	GLU
1	C	95	ARG
1	C	113	CYS
1	C	122	ARG
1	C	124	ASP
1	C	150	ARG
1	C	192	GLU
1	C	195	ARG
1	C	198	LEU
1	C	199	GLU
1	C	219	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	239	LEU
1	C	257	ARG
1	C	261	ARG
1	C	282	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	70	GLN
1	A	96	HIS
1	A	130	GLN
1	A	143	GLN
1	A	238	GLN
1	B	12	GLN
1	B	130	GLN
1	B	143	GLN
1	C	12	GLN
1	C	98	HIS
1	C	139	GLN
1	C	151	ASN
1	C	282	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	270/400 (67%)	0.44	11 (4%) 41 44	13, 31, 61, 85	0
1	B	261/400 (65%)	0.58	13 (4%) 32 36	19, 41, 74, 124	0
1	C	254/400 (63%)	1.65	76 (29%) 1 0	48, 88, 121, 149	0
2	D	26/26 (100%)	0.09	2 (7%) 16 17	34, 67, 110, 118	0
2	E	26/26 (100%)	0.10	0 100 100	29, 64, 79, 85	0
3	F	26/26 (100%)	0.61	3 (11%) 6 6	68, 98, 111, 116	0
All	All	863/1278 (67%)	0.82	105 (12%) 5 5	13, 50, 110, 149	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	75	LEU	13.0
1	B	191	PHE	8.9
1	B	242	ARG	8.7
1	C	23	PHE	8.5
1	C	110	LEU	7.9
1	C	22	VAL	7.9
1	A	33	SER	7.3
1	C	159	ARG	6.6
1	C	46	ARG	6.5
1	C	129	TRP	6.1
1	C	109	ARG	6.0
1	C	73	LEU	6.0
1	C	60	LEU	5.8
1	C	125	LEU	5.8
1	C	271	LEU	5.7
1	C	253	PHE	5.4
1	C	290	PRO	5.3
1	C	44	ALA	5.3
1	C	72	PRO	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	147	ASN	4.7
1	C	220	LEU	4.6
1	C	92	GLU	4.6
1	C	19	ARG	4.4
1	C	47	ILE	4.3
1	A	247	GLU	4.3
1	C	122	ARG	4.2
1	C	40	PHE	4.2
1	C	71	GLU	4.2
1	C	126	GLY	4.2
1	C	155	LYS	4.0
1	A	291	LYS	4.0
1	C	90	ARG	3.9
3	F	28	DG	3.8
1	C	91	GLU	3.7
1	C	21	LEU	3.7
1	A	245	GLY	3.7
1	C	20	ALA	3.7
1	C	280	TRP	3.7
1	C	18	CYS	3.7
2	D	16	DT	3.7
1	C	48	SER	3.7
1	A	249	GLY	3.7
1	C	63	LEU	3.7
1	C	58	LEU	3.6
3	F	2	DG	3.6
1	C	64	PRO	3.6
1	A	32	VAL	3.5
1	A	274	ARG	3.5
1	C	27	VAL	3.5
1	A	94	PRO	3.5
1	A	248	SER	3.4
1	A	246	SER	3.4
1	C	165	LEU	3.4
2	D	13	DC	3.4
1	C	287	PRO	3.3
1	C	69	GLN	3.3
1	C	152	LEU	3.2
1	C	149	LEU	3.2
1	C	34	ARG	3.2
3	F	1	DC	3.2
1	C	62	PRO	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	34	ARG	3.2
1	C	272	GLN	3.1
1	C	9	LEU	2.9
1	B	290	PRO	2.9
1	B	155	LYS	2.9
1	C	89	PRO	2.9
1	C	191	PHE	2.9
1	B	244	TYR	2.9
1	C	74	ALA	2.8
1	C	26	CYS	2.8
1	C	13	PHE	2.7
1	C	87	LEU	2.7
1	C	281	PHE	2.7
1	C	197	VAL	2.6
1	B	64	PRO	2.6
1	B	280	TRP	2.6
1	C	78	ARG	2.6
1	B	258	ALA	2.5
1	C	100	ARG	2.5
1	C	105	PRO	2.5
1	C	278	THR	2.5
1	C	32	VAL	2.4
1	C	61	SER	2.4
1	C	279	ILE	2.4
1	C	25	GLY	2.4
1	C	56	LEU	2.4
1	C	166	LEU	2.3
1	C	123	TRP	2.3
1	B	69	GLN	2.3
1	C	38	VAL	2.3
1	B	161	ILE	2.3
1	C	170	PHE	2.2
1	C	177	TYR	2.1
1	B	65	GLY	2.1
1	B	241	GLY	2.1
1	C	194	ALA	2.1
1	B	190	PRO	2.1
1	C	270	SER	2.1
1	C	192	GLU	2.1
1	C	173	GLY	2.1
1	C	254	ALA	2.0
1	C	162	CYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	132	GLY	2.0
1	C	263	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.