Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:49 AM GMT

PDB ID	:	3JTS
Title	:	GY9-Mamu-A*02-hb2m
Authors	:	Dai, L.; Feng, Y.; Qi, J.; Gao, G.F.
Deposited on	:	2009-09-14
Resolution	:	2.80 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
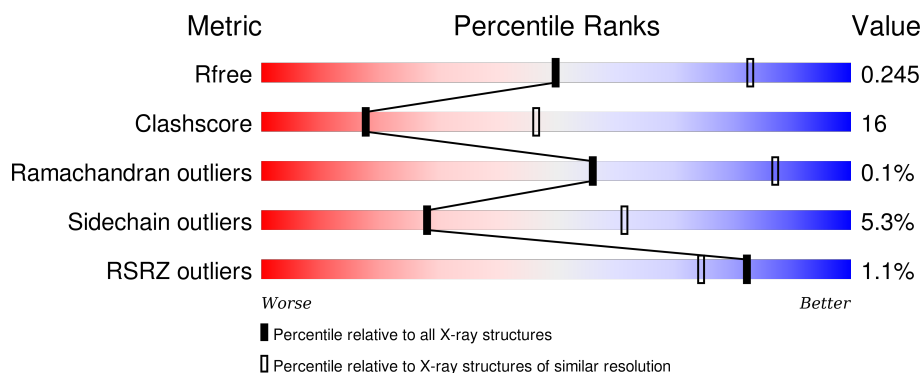
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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	276	67% 29% •
1	D	276	70% 27% •
1	G	276	63% 34% •
2	B	119	63% 18% • 17%
2	E	119	66% 13% • 17%

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Mol	Chain	Length	Quality of chain
2	H	119	58% 24% 17%
3	C	9	56% 33% 11%
3	F	9	56% 44%
3	I	9	44% 56%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9659 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 MHC class I Mamu-A*02.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total 2262	C 1402	N 415	O 435	S 10	0	0	0
1	D	276	Total 2262	C 1402	N 415	O 435	S 10	0	0	0
1	G	276	Total 2262	C 1402	N 415	O 435	S 10	0	0	0

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total 829	C 528	N 140	O 158	S 3	0	0	0
2	E	99	Total 829	C 528	N 140	O 158	S 3	0	0	0
2	H	99	Total 829	C 528	N 140	O 158	S 3	0	0	0

- Molecule 3 is a protein called peptide of Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total 71	C 44	N 11	O 16	0	0	0
3	F	9	Total 71	C 44	N 11	O 16	0	0	0
3	I	9	Total 71	C 44	N 11	O 16	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	37	Total 37	O 37		0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	14	Total 14	O 14	0	0
4	C	1	Total 1	O 1	0	0
4	D	34	Total 34	O 34	0	0
4	E	15	Total 15	O 15	0	0
4	F	2	Total 2	O 2	0	0
4	G	49	Total 49	O 49	0	0
4	H	20	Total 20	O 20	0	0
4	I	1	Total 1	O 1	0	0

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: MHC class I Mamu-A*02
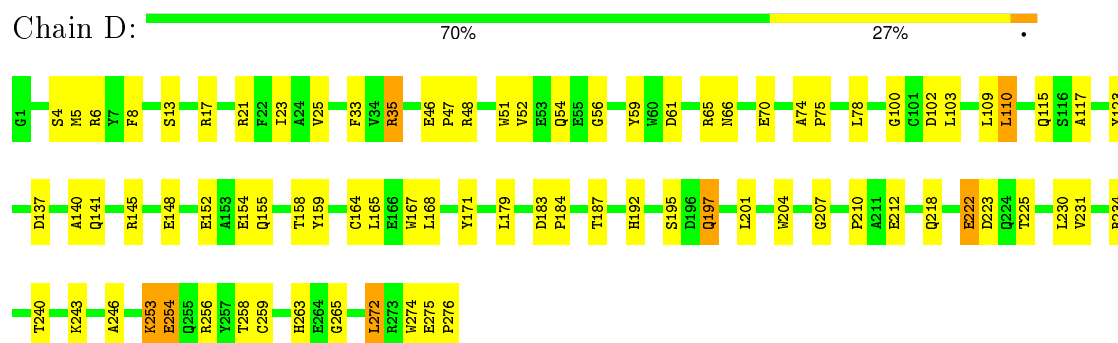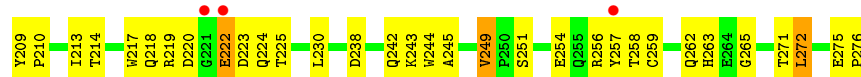
- Molecule 1: MHC class I Mamu-A*02

- Molecule 1: MHC class I Mamu-A*02

• Molecule 2: Beta-2-microglobulin
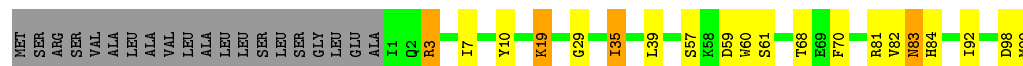
Chain B:

• Molecule 2: Beta-2-microglobulin

Chain E:

• Molecule 2: Beta-2-microglobulin

Chain H:

• Molecule 3: peptide of Gag-Pol polyprotein

Chain C:

• Molecule 3: peptide of Gag-Pol polyprotein
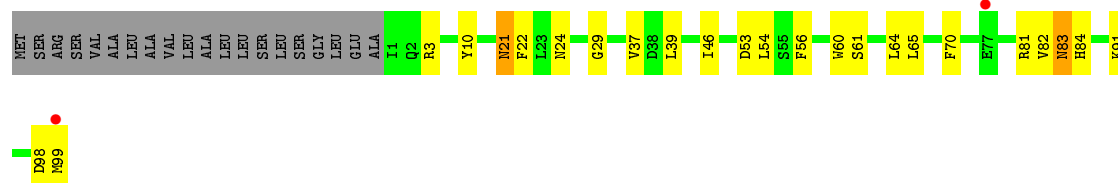
Chain F:

• Molecule 3: peptide of Gag-Pol polyprotein

Chain I:
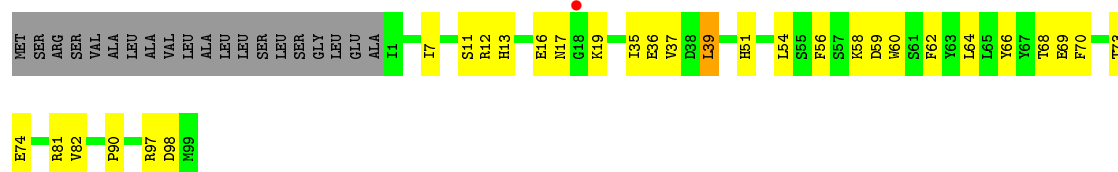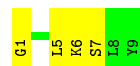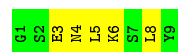
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	123.96Å 110.33Å 100.09Å 90.00° 114.32° 90.00°	Depositor
Resolution (Å)	38.70 – 2.80 38.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.70-2.80) 99.8 (38.70-2.80)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$<I/\sigma(I)>$ [1]	3.99 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.197 , 0.248 0.189 , 0.245	Depositor DCC
R_{free} test set	1526 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	37.9	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Outliers	0 of 30210 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9659	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.36	0/2325	0.55	5/3156 (0.2%)
1	D	0.38	0/2325	0.49	0/3156
1	G	0.37	0/2325	0.49	0/3156
2	B	0.28	0/852	0.43	0/1152
2	E	0.31	0/852	0.45	0/1152
2	H	0.32	0/852	0.47	0/1152
3	C	0.32	0/71	0.97	1/92 (1.1%)
3	F	0.52	0/71	0.68	0/92
3	I	0.34	0/71	0.43	0/92
All	All	0.35	0/9744	0.50	6/13200 (0.0%)

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	GLU	N-CA-CB	6.98	123.17	110.60
1	A	163	GLU	N-CA-C	-6.86	92.48	111.00
1	A	164	CYS	CA-CB-SG	5.96	124.73	114.00
3	C	7	SER	CB-CA-C	5.80	121.12	110.10
1	A	162	GLY	C-N-CA	5.57	135.63	121.70
1	A	162	GLY	O-C-N	-5.25	114.30	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	GLY	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	2262	0	2102	75	0
1	D	2262	0	2101	68	0
1	G	2262	0	2101	93	1
2	B	829	0	794	21	0
2	E	829	0	794	16	0
2	H	829	0	794	21	0
3	C	71	0	71	4	0
3	F	71	0	71	6	0
3	I	71	0	71	14	0
4	A	37	0	0	5	0
4	B	14	0	0	0	0
4	C	1	0	0	0	0
4	D	34	0	0	0	0
4	E	15	0	0	0	0
4	F	2	0	0	0	0
4	G	49	0	0	3	0
4	H	20	0	0	1	0
4	I	1	0	0	0	0
All	All	9659	0	8899	291	1

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 16.

All (291) 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:G:219:ARG:NH2	1:G:257:TYR:CZ	2.25	1.04
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.55	0.88
1:G:196:ASP:O	1:G:197:GLN:HG3	1.74	0.85
1:G:194:VAL:CG2	1:G:198:GLU:O	2.24	0.84
2:H:7:ILE:HD12	2:H:82:VAL:HG21	1.56	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:VAL:HB	1:G:257:TYR:HE2	1.42	0.83
1:G:249:VAL:HB	1:G:257:TYR:CE2	2.14	0.82
1:D:263:HIS:CD2	1:D:265:GLY:H	1.96	0.82
1:D:33:PHE:HB2	1:D:52:VAL:HG21	1.61	0.81
1:A:145:ARG:HG2	4:A:284:HOH:O	1.79	0.81
1:G:198:GLU:HA	1:G:249:VAL:O	1.81	0.80
1:G:219:ARG:NH2	1:G:257:TYR:CE2	2.50	0.79
1:G:194:VAL:HG22	1:G:198:GLU:O	1.84	0.79
1:A:33:PHE:HB2	1:A:52:VAL:HG21	1.65	0.78
2:H:81:ARG:HD3	2:H:90:PRO:HB3	1.64	0.78
1:G:219:ARG:HH11	1:G:256:ARG:NE	1.82	0.78
3:I:5:LEU:HG	3:I:6:LYS:N	1.99	0.77
1:A:156:HIS:HD2	3:C:3:GLU:OE1	1.68	0.77
2:B:21:ASN:ND2	2:B:22:PHE:H	1.83	0.76
2:B:3:ARG:HH21	2:B:61:SER:HB3	1.51	0.76
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.67	0.75
2:E:7:ILE:HD12	2:E:82:VAL:HG21	1.69	0.75
1:D:103:LEU:HD13	1:D:165:LEU:HD22	1.66	0.75
1:A:101:CYS:CB	1:A:164:CYS:SG	2.74	0.75
1:G:194:VAL:HG23	1:G:195:SER:H	1.53	0.73
3:F:5:LEU:HD23	3:F:6:LYS:H	1.52	0.72
1:G:156:HIS:HD2	3:I:3:GLU:OE1	1.71	0.72
1:G:64:THR:HG22	1:G:68:LYS:HE2	1.71	0.72
1:A:187:THR:HB	1:A:272:LEU:HD21	1.72	0.72
1:A:162:GLY:O	1:A:166:GLU:HG3	1.90	0.71
1:A:219:ARG:HG3	1:A:219:ARG:O	1.90	0.71
1:G:194:VAL:HG23	1:G:198:GLU:O	1.88	0.70
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.73	0.70
1:A:204:TRP:HZ2	2:B:99:MET:HB3	1.57	0.70
1:G:33:PHE:HB2	1:G:52:VAL:HG21	1.74	0.69
1:D:259:CYS:HB3	1:D:272:LEU:CD1	2.22	0.69
2:E:29:GLY:HA2	2:E:61:SER:HB2	1.74	0.69
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.73	0.69
1:A:163:GLU:HB2	4:A:282:HOH:O	1.92	0.69
1:G:263:HIS:HD2	1:G:265:GLY:H	1.39	0.68
1:A:259:CYS:HB3	1:A:272:LEU:CD1	2.23	0.67
2:B:99:MET:O	2:B:99:MET:HG3	1.93	0.67
1:D:21:ARG:HD2	1:D:23:ILE:HD11	1.77	0.67
1:D:187:THR:HB	1:D:272:LEU:HD21	1.76	0.66
2:B:39:LEU:O	2:B:46:ILE:HG12	1.95	0.66
1:A:145:ARG:N	4:A:284:HOH:O	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:TRP:CE3	1:A:18:TRP:HA	2.31	0.66
1:D:35:ARG:NH2	1:D:48:ARG:HH21	1.94	0.65
2:H:39:LEU:HD23	2:H:68:THR:HG22	1.79	0.65
1:G:14:ARG:CG	1:G:15:PRO:HD2	2.26	0.65
1:A:18:TRP:HA	1:A:18:TRP:HE3	1.62	0.64
1:G:219:ARG:HH11	1:G:256:ARG:CZ	2.10	0.64
1:A:272:LEU:HD12	1:A:272:LEU:H	1.63	0.64
1:A:210:PRO:O	1:A:263:HIS:HE1	1.82	0.63
1:G:44:ARG:NH2	1:G:61:ASP:OD1	2.31	0.63
1:G:263:HIS:CD2	1:G:265:GLY:H	2.16	0.63
1:A:35:ARG:HE	1:A:48:ARG:HE	1.46	0.63
1:D:47:PRO:O	1:D:48:ARG:HD3	1.98	0.63
1:A:68:LYS:O	1:A:72:GLN:HG2	2.01	0.61
1:A:9:TYR:HB2	1:A:97:ARG:HB3	1.83	0.61
3:C:6:LYS:O	3:C:7:SER:HB2	2.00	0.60
1:G:218:GLN:HA	1:G:222:GLU:O	2.01	0.60
1:D:263:HIS:HD2	1:D:265:GLY:H	1.46	0.60
1:A:6:ARG:HD3	1:A:100:GLY:HA3	1.83	0.60
1:G:249:VAL:CB	1:G:257:TYR:CE2	2.85	0.60
1:D:21:ARG:HH11	1:D:23:ILE:HD11	1.67	0.60
1:G:189:VAL:HG23	1:G:272:LEU:HD22	1.82	0.60
1:G:251:SER:HA	1:G:254:GLU:OE1	2.01	0.59
1:D:51:TRP:CZ2	1:D:179:LEU:HD11	2.37	0.59
1:D:148:GLU:HB3	3:I:8:LEU:HD13	1.84	0.59
1:G:51:TRP:CE3	1:G:52:VAL:HG22	2.38	0.59
2:B:29:GLY:HA2	2:B:61:SER:CB	2.32	0.59
2:H:73:THR:HG22	2:H:74:GLU:H	1.66	0.59
1:G:190:THR:HG21	4:G:320:HOH:O	2.02	0.59
3:I:5:LEU:CG	3:I:6:LYS:N	2.66	0.59
1:A:204:TRP:CZ2	2:B:99:MET:HB3	2.36	0.59
1:A:263:HIS:CD2	1:A:265:GLY:H	2.21	0.59
1:A:79:ARG:HG2	1:A:82:ARG:NH2	2.18	0.58
2:H:54:LEU:HD11	2:H:62:PHE:CD2	2.38	0.58
1:A:135:ALA:HB1	1:A:140:ALA:HB3	1.85	0.58
1:G:14:ARG:NH2	1:G:19:GLU:HG2	2.17	0.58
1:G:109:LEU:HD11	1:G:111:ARG:O	2.04	0.57
1:D:154:GLU:O	1:D:158:THR:HG22	2.04	0.57
1:G:84:TYR:HB3	1:G:139:ALA:HB1	1.87	0.57
1:G:51:TRP:CZ3	1:G:52:VAL:HG22	2.39	0.57
2:H:17:ASN:ND2	2:H:97:ARG:HH22	2.03	0.56
1:G:249:VAL:CG1	1:G:257:TYR:CE2	2.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:29:GLY:HA2	2:E:61:SER:CB	2.36	0.56
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.41	0.56
1:D:197:GLN:H	1:D:197:GLN:HE21	1.52	0.56
1:D:35:ARG:HD3	1:D:46:GLU:OE1	2.06	0.55
1:D:4:SER:HB3	1:D:102:ASP:HA	1.88	0.55
1:G:47:PRO:HB3	1:G:60:TRP:CH2	2.42	0.55
1:G:62:ARG:HH12	1:G:167:TRP:HZ2	1.55	0.55
1:D:197:GLN:H	1:D:197:GLN:NE2	2.05	0.55
1:A:13:SER:CB	1:A:78:LEU:HD13	2.34	0.54
1:D:66:ASN:O	1:D:70:GLU:HG2	2.08	0.54
1:G:242:GLN:O	1:G:243:LYS:HB2	2.07	0.54
1:D:8:PHE:HB2	1:D:25:VAL:HG23	1.90	0.54
1:G:259:CYS:HB3	1:G:272:LEU:HD13	1.90	0.54
1:A:129:ASP:O	1:A:131:ARG:HG3	2.08	0.54
3:I:4:ASN:ND2	3:I:6:LYS:HE3	2.23	0.54
2:E:59:ASP:O	2:E:60:TRP:HB2	2.07	0.54
1:G:70:GLU:OE1	3:I:5:LEU:HD13	2.08	0.54
1:A:28:VAL:HG23	1:A:33:PHE:CE1	2.44	0.53
1:A:82:ARG:NH1	1:A:89:GLU:HG3	2.23	0.53
2:H:54:LEU:HA	2:H:64:LEU:HD21	1.90	0.53
1:D:109:LEU:HB2	1:D:165:LEU:CD1	2.39	0.53
1:G:82:ARG:HD2	1:G:88:SER:O	2.09	0.53
2:B:83:ASN:HD22	2:B:84:HIS:N	2.07	0.52
1:D:51:TRP:CZ2	1:D:179:LEU:HD21	2.45	0.52
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.44	0.52
2:B:3:ARG:NH2	2:B:61:SER:HB3	2.21	0.52
1:D:195:SER:HB2	1:D:197:GLN:HE22	1.75	0.52
1:A:56:GLY:O	1:A:59:TYR:HB3	2.10	0.52
1:A:115:GLN:HG2	1:A:125:ALA:HB1	1.92	0.52
1:A:234:ARG:HD2	2:B:10:TYR:CE1	2.44	0.52
2:E:19:LYS:N	2:E:19:LYS:HD2	2.25	0.51
1:A:107:GLY:O	1:A:108:ARG:HG3	2.11	0.51
1:G:144:GLN:O	1:G:148:GLU:HB2	2.10	0.51
1:G:219:ARG:NH1	1:G:256:ARG:NE	2.54	0.51
2:H:73:THR:HG22	2:H:74:GLU:N	2.25	0.51
1:G:124:ILE:HD11	1:G:133:TRP:HB3	1.92	0.51
1:D:145:ARG:HB2	3:I:6:LYS:HB3	1.93	0.51
1:D:70:GLU:OE2	3:F:5:LEU:HD22	2.09	0.51
1:D:6:ARG:HD3	1:D:100:GLY:HA3	1.93	0.51
1:G:62:ARG:NH1	1:G:167:TRP:HZ2	2.08	0.51
1:D:61:ASP:O	1:D:65:ARG:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:LEU:HA	1:D:165:LEU:HD11	1.92	0.51
1:A:142:ASN:C	4:A:284:HOH:O	2.49	0.50
1:A:137:ASP:OD2	1:A:138:MET:N	2.44	0.50
1:G:6:ARG:HD3	1:G:100:GLY:HA3	1.92	0.50
1:G:195:SER:O	1:G:198:GLU:HB2	2.12	0.50
1:G:73:ASN:HD22	3:I:5:LEU:HD11	1.76	0.50
3:I:5:LEU:HD23	3:I:6:LYS:H	1.75	0.50
1:A:152:GLU:OE2	3:C:7:SER:HB2	2.11	0.50
2:E:81:ARG:HG3	2:E:92:ILE:HG12	1.93	0.50
1:D:274:TRP:CD2	1:D:276:PRO:HD3	2.47	0.50
1:D:109:LEU:HB2	1:D:165:LEU:HD11	1.93	0.50
1:G:219:ARG:NH1	1:G:256:ARG:HE	2.09	0.50
1:G:219:ARG:NH1	1:G:256:ARG:NH2	2.60	0.49
1:A:89:GLU:CD	1:A:89:GLU:N	2.65	0.49
1:G:202:ARG:HD3	1:G:244:TRP:CD2	2.47	0.49
3:C:4:ASN:ND2	3:C:6:LYS:HD3	2.27	0.49
1:D:13:SER:HB3	1:D:78:LEU:HD13	1.92	0.49
1:D:204:TRP:CH2	2:E:99:MET:HA	2.47	0.49
1:D:33:PHE:HB2	1:D:52:VAL:CG2	2.39	0.49
1:A:154:GLU:O	1:A:158:THR:HG22	2.12	0.49
2:H:17:ASN:HD21	2:H:97:ARG:HH22	1.60	0.49
1:A:33:PHE:O	1:A:48:ARG:N	2.42	0.49
1:G:154:GLU:HG3	1:G:157:ARG:HH22	1.77	0.49
1:G:66:ASN:O	1:G:70:GLU:HG2	2.13	0.49
1:A:117:ALA:HB2	2:B:60:TRP:CD2	2.48	0.49
1:D:210:PRO:O	1:D:263:HIS:HE1	1.96	0.49
1:D:109:LEU:CA	1:D:165:LEU:HD11	2.43	0.48
1:A:263:HIS:HD2	1:A:265:GLY:H	1.60	0.48
1:G:14:ARG:HG2	1:G:15:PRO:HD2	1.95	0.48
2:B:21:ASN:ND2	2:B:22:PHE:N	2.58	0.48
3:I:8:LEU:N	3:I:8:LEU:HD12	2.29	0.48
1:G:82:ARG:HG2	1:G:82:ARG:HH11	1.77	0.48
2:B:83:ASN:HD22	2:B:84:HIS:H	1.61	0.48
1:D:56:GLY:O	1:D:59:TYR:HB3	2.14	0.48
2:H:59:ASP:O	2:H:60:TRP:HB2	2.13	0.48
1:A:261:VAL:HB	1:A:270:LEU:HB2	1.96	0.48
1:A:124:ILE:HD12	1:A:134:THR:O	2.14	0.48
1:G:222:GLU:HG2	1:G:224:GLN:HE22	1.78	0.48
1:A:35:ARG:HG3	2:B:53:ASP:CG	2.34	0.48
2:B:54:LEU:HA	2:B:64:LEU:HD21	1.95	0.48
1:G:37:ASP:HB3	1:G:40:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:GLN:HA	1:D:222:GLU:O	2.15	0.47
2:E:35:ILE:HD13	2:E:83:ASN:O	2.14	0.47
1:A:87:GLN:NE2	1:A:93:HIS:CE1	2.83	0.47
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.49	0.47
1:A:143:THR:O	1:A:146:LYS:HB2	2.15	0.47
3:I:5:LEU:CD2	3:I:6:LYS:H	2.28	0.47
1:A:33:PHE:C	1:A:48:ARG:HB2	2.35	0.47
1:D:234:ARG:HD2	2:E:10:TYR:CE1	2.50	0.47
1:A:271:THR:O	1:A:271:THR:HG22	2.15	0.47
1:G:196:ASP:N	4:G:277:HOH:O	2.48	0.47
3:I:5:LEU:HG	3:I:6:LYS:H	1.80	0.47
1:D:253:LYS:HG3	1:D:256:ARG:HD3	1.97	0.47
2:E:35:ILE:CD1	2:E:82:VAL:HG13	2.46	0.46
1:G:111:ARG:HG3	1:G:112:GLY:N	2.29	0.46
1:A:81:LEU:HA	1:A:84:TYR:CD2	2.50	0.46
1:G:238:ASP:HB3	2:H:12:ARG:HD3	1.98	0.46
1:G:163:GLU:O	1:G:167:TRP:CD1	2.69	0.46
1:D:137:ASP:O	1:D:141:GLN:HG3	2.16	0.46
2:E:3:ARG:NH1	2:E:3:ARG:HB3	2.30	0.46
1:D:152:GLU:OE2	3:F:7:SER:HB2	2.15	0.46
1:G:189:VAL:HG23	1:G:272:LEU:CD2	2.46	0.46
1:D:192:HIS:CE1	2:E:98:ASP:CG	2.89	0.46
1:G:154:GLU:HG3	1:G:157:ARG:NH2	2.30	0.46
1:G:58:GLU:HG3	4:G:286:HOH:O	2.15	0.45
2:H:39:LEU:HD23	2:H:68:THR:CG2	2.45	0.45
1:G:168:LEU:O	1:G:172:LEU:HG	2.17	0.45
2:H:58:LYS:HE2	2:H:58:LYS:HB3	1.75	0.45
1:D:230:LEU:HD22	1:D:243:LYS:HE3	1.98	0.45
1:G:272:LEU:N	1:G:272:LEU:CD1	2.80	0.45
1:A:89:GLU:CD	1:A:89:GLU:H	2.20	0.45
1:D:197:GLN:N	1:D:197:GLN:NE2	2.65	0.45
1:G:154:GLU:O	1:G:158:THR:HG22	2.16	0.45
1:A:84:TYR:HB3	1:A:139:ALA:HB1	1.99	0.45
1:D:183:ASP:HA	1:D:184:PRO:HD2	1.77	0.45
1:D:195:SER:HB2	1:D:197:GLN:NE2	2.32	0.45
1:A:144:GLN:N	4:A:284:HOH:O	2.50	0.45
3:I:5:LEU:CG	3:I:6:LYS:H	2.29	0.45
1:G:14:ARG:HG3	1:G:15:PRO:HD2	1.99	0.45
3:I:5:LEU:O	3:I:6:LYS:HB2	2.17	0.45
1:A:17:ARG:O	1:A:18:TRP:C	2.56	0.45
1:A:231:VAL:HG21	1:A:244:TRP:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:HD2	1:A:48:ARG:HA	1.66	0.44
1:G:35:ARG:HG2	1:G:36:PHE:N	2.27	0.44
1:D:275:GLU:OE2	1:D:275:GLU:HA	2.18	0.44
1:D:259:CYS:HB3	1:D:272:LEU:HD13	1.97	0.44
1:A:82:ARG:HG2	1:A:87:GLN:O	2.18	0.44
1:D:167:TRP:CD1	3:F:1:GLY:HA3	2.53	0.44
1:A:14:ARG:NH1	1:A:21:ARG:HG3	2.31	0.44
1:G:82:ARG:NH1	1:G:89:GLU:HG3	2.32	0.44
2:E:39:LEU:HD23	2:E:68:THR:HG22	1.98	0.44
1:G:64:THR:O	1:G:68:LYS:HG3	2.17	0.44
1:A:252:GLY:N	1:A:254:GLU:OE2	2.50	0.44
1:A:187:THR:HB	1:A:272:LEU:CD2	2.44	0.44
1:D:254:GLU:HG3	1:D:274:TRP:CE3	2.53	0.44
1:D:5:MET:HB2	1:D:168:LEU:HD13	2.00	0.44
1:D:167:TRP:HB3	1:D:171:TYR:CE2	2.53	0.44
1:G:217:TRP:O	1:G:223:ASP:HA	2.18	0.44
2:E:83:ASN:HD22	2:E:84:HIS:N	2.16	0.44
1:D:23:ILE:HD12	1:D:23:ILE:N	2.32	0.44
1:D:155:GLN:HA	1:D:158:THR:HG22	1.99	0.44
1:G:131:ARG:HG2	1:G:157:ARG:NH2	2.33	0.44
1:D:201:LEU:O	1:D:246:ALA:HA	2.18	0.44
1:G:209:TYR:CG	1:G:210:PRO:HA	2.53	0.44
1:G:64:THR:CG2	1:G:68:LYS:HE2	2.45	0.44
2:H:16:GLU:OE1	2:H:19:LYS:HG3	2.18	0.44
1:D:167:TRP:NE1	3:F:1:GLY:HA3	2.33	0.43
1:D:207:GLY:HA2	1:D:240:THR:OG1	2.18	0.43
1:G:275:GLU:HA	1:G:276:PRO:HD2	1.87	0.43
1:G:163:GLU:CG	1:G:167:TRP:HE1	2.31	0.43
1:G:163:GLU:O	1:G:167:TRP:HD1	2.01	0.43
1:G:223:ASP:HB2	1:G:225:THR:HG23	2.00	0.43
2:H:36:GLU:HG2	4:H:165:HOH:O	2.18	0.43
1:G:230:LEU:HD23	1:G:245:ALA:HB2	1.99	0.43
1:A:185:PRO:HB3	1:A:208:PHE:HB3	2.00	0.43
1:D:35:ARG:CZ	1:D:48:ARG:HH21	2.32	0.43
1:G:115:GLN:HE21	1:G:115:GLN:HB3	1.53	0.43
1:D:165:LEU:HA	1:D:165:LEU:HD23	1.86	0.43
1:A:14:ARG:HD3	1:A:21:ARG:HB2	2.00	0.43
1:A:74:ALA:N	1:A:75:PRO:HD2	2.34	0.43
1:D:123:TYR:CZ	1:D:140:ALA:HA	2.53	0.42
1:G:28:VAL:HG23	1:G:33:PHE:CE1	2.54	0.42
1:G:192:HIS:HE1	2:H:98:ASP:OD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.55	0.42
1:A:63:GLU:O	1:A:67:MET:HG2	2.20	0.42
1:A:79:ARG:HH11	1:A:79:ARG:HG3	1.84	0.42
1:G:183:ASP:HA	1:G:184:PRO:HD2	1.89	0.42
1:G:219:ARG:HG3	1:G:220:ASP:CG	2.40	0.42
1:G:197:GLN:HA	1:G:251:SER:OG	2.20	0.42
1:D:6:ARG:HH21	1:D:102:ASP:CG	2.22	0.42
1:A:128:GLU:O	1:A:130:LEU:HG	2.20	0.42
2:E:35:ILE:HD11	2:E:82:VAL:HG13	2.02	0.42
1:G:103:LEU:HD13	1:G:165:LEU:HD22	2.02	0.42
1:A:183:ASP:HA	1:A:184:PRO:HD2	1.92	0.42
1:A:187:THR:HA	1:A:204:TRP:O	2.20	0.41
1:G:111:ARG:HG2	1:G:113:TYR:CZ	2.55	0.41
1:G:8:PHE:HD2	2:H:56:PHE:CE2	2.38	0.41
1:G:182:ALA:HA	1:G:209:TYR:O	2.20	0.41
2:H:35:ILE:HG12	2:H:36:GLU:N	2.35	0.41
1:G:21:ARG:NE	1:G:23:ILE:HD11	2.34	0.41
1:A:79:ARG:HG2	1:A:82:ARG:HH21	1.85	0.41
1:G:203:CYS:HB2	1:G:217:TRP:CZ2	2.55	0.41
1:D:159:TYR:CE2	1:D:164:CYS:HB2	2.56	0.41
1:G:249:VAL:HG11	1:G:257:TYR:CE2	2.54	0.41
1:G:189:VAL:CG2	1:G:272:LEU:HD22	2.51	0.41
2:H:37:VAL:HB	2:H:66:TYR:CZ	2.56	0.41
1:D:51:TRP:HZ2	1:D:179:LEU:HD21	1.83	0.41
2:H:12:ARG:HG2	2:H:13:HIS:CE1	2.54	0.41
1:G:213:ILE:HG12	1:G:214:THR:H	1.85	0.41
1:D:223:ASP:HB3	1:D:225:THR:HG23	2.02	0.41
1:A:37:ASP:HB3	1:A:40:ALA:HB2	2.02	0.41
2:B:81:ARG:HA	2:B:91:LYS:O	2.20	0.41
1:A:231:VAL:HG13	1:A:244:TRP:CZ2	2.55	0.41
1:A:76:VAL:HG13	1:A:79:ARG:NH2	2.35	0.41
1:G:82:ARG:NH1	1:G:82:ARG:HG2	2.36	0.41
1:A:258:THR:HG23	1:A:271:THR:HG23	2.03	0.41
1:D:152:GLU:OE2	3:F:7:SER:CB	2.69	0.41
1:A:8:PHE:HB3	2:B:56:PHE:CE1	2.55	0.40
1:D:110:LEU:O	1:D:110:LEU:HG	2.19	0.40
1:G:259:CYS:O	1:G:271:THR:HA	2.21	0.40
1:A:259:CYS:HB3	1:A:272:LEU:HD12	2.02	0.40
1:D:74:ALA:N	1:D:75:PRO:HD2	2.37	0.40
1:D:263:HIS:CD2	1:D:265:GLY:N	2.78	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:194:VAL:O	1:G:196:ASP:OD2[2_554]	2.19	0.01

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	274/276 (99%)	263 (96%)	10 (4%)	1 (0%)	39	74
1	D	274/276 (99%)	254 (93%)	20 (7%)	0	100	100
1	G	274/276 (99%)	253 (92%)	21 (8%)	0	100	100
2	B	97/119 (82%)	94 (97%)	3 (3%)	0	100	100
2	E	97/119 (82%)	92 (95%)	5 (5%)	0	100	100
2	H	97/119 (82%)	88 (91%)	9 (9%)	0	100	100
3	C	7/9 (78%)	4 (57%)	3 (43%)	0	100	100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	I	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
All	All	1134/1212 (94%)	1059 (93%)	74 (6%)	1 (0%)	56	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLY

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	233/233 (100%)	221 (95%)	12 (5%)	29	62
1	D	233/233 (100%)	220 (94%)	13 (6%)	26	59
1	G	233/233 (100%)	220 (94%)	13 (6%)	26	59
2	B	94/109 (86%)	90 (96%)	4 (4%)	35	70
2	E	94/109 (86%)	88 (94%)	6 (6%)	22	52
2	H	94/109 (86%)	89 (95%)	5 (5%)	28	61
3	C	8/8 (100%)	8 (100%)	0	100	100
3	F	8/8 (100%)	8 (100%)	0	100	100
3	I	8/8 (100%)	8 (100%)	0	100	100
All	All	1005/1050 (96%)	952 (95%)	53 (5%)	28	61

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	18	TRP
1	A	21	ARG
1	A	48	ARG
1	A	114	HIS
1	A	157	ARG
1	A	165	LEU
1	A	197	GLN
1	A	219	ARG
1	A	231	VAL
1	A	254	GLU
1	A	272	LEU
2	B	21	ASN
2	B	70	PHE
2	B	83	ASN
2	B	98	ASP
1	D	17	ARG
1	D	35	ARG
1	D	54	GLN
1	D	110	LEU
1	D	115	GLN
1	D	197	GLN
1	D	212	GLU
1	D	222	GLU

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Mol	Chain	Res	Type
1	D	231	VAL
1	D	253	LYS
1	D	254	GLU
1	D	258	THR
1	D	272	LEU
2	E	3	ARG
2	E	19	LYS
2	E	35	ILE
2	E	57	SER
2	E	70	PHE
2	E	83	ASN
1	G	14	ARG
1	G	18	TRP
1	G	25	VAL
1	G	82	ARG
1	G	115	GLN
1	G	148	GLU
1	G	186	LYS
1	G	197	GLN
1	G	222	GLU
1	G	249	VAL
1	G	258	THR
1	G	262	GLN
1	G	272	LEU
2	H	11	SER
2	H	39	LEU
2	H	51	HIS
2	H	69	GLU
2	H	70	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	87	GLN
1	A	156	HIS
1	A	224	GLN
1	A	226	GLN
1	A	255	GLN
1	A	262	GLN
1	A	263	HIS
2	B	21	ASN

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Mol	Chain	Res	Type
2	B	31	HIS
2	B	83	ASN
2	B	89	GLN
3	C	4	ASN
1	D	32	GLN
1	D	54	GLN
1	D	73	ASN
1	D	80	ASN
1	D	86	ASN
1	D	115	GLN
1	D	127	ASN
1	D	156	HIS
1	D	192	HIS
1	D	197	GLN
1	D	226	GLN
1	D	255	GLN
1	D	263	HIS
2	E	2	GLN
2	E	83	ASN
1	G	72	GLN
1	G	96	GLN
1	G	114	HIS
1	G	156	HIS
1	G	191	HIS
1	G	192	HIS
1	G	224	GLN
1	G	226	GLN
1	G	255	GLN
1	G	263	HIS
2	H	13	HIS
2	H	17	ASN
3	I	4	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	276/276 (100%)	-0.24	4 (1%)	78	69	19, 36, 62, 78	0
1	D	276/276 (100%)	-0.28	0	100	100	20, 35, 59, 80	0
1	G	276/276 (100%)	-0.22	6 (2%)	65	54	21, 34, 64, 79	0
2	B	99/119 (83%)	-0.23	2 (2%)	68	58	28, 44, 65, 79	0
2	E	99/119 (83%)	-0.58	0	100	100	21, 31, 48, 55	0
2	H	99/119 (83%)	-0.16	1 (1%)	84	77	27, 41, 73, 85	0
3	C	9/9 (100%)	0.45	0	100	100	28, 45, 57, 64	0
3	F	9/9 (100%)	0.04	0	100	100	29, 36, 51, 58	0
3	I	9/9 (100%)	0.10	0	100	100	26, 47, 57, 63	0
All	All	1152/1212 (95%)	-0.26	13 (1%)	82	74	19, 36, 63, 85	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	257	TYR	3.8
1	G	221	GLY	3.1
2	B	99	MET	3.0
1	A	222	GLU	3.0
1	G	16	GLY	2.7
1	A	142	ASN	2.7
1	G	196	ASP	2.6
1	A	85	TYR	2.6
2	B	77	GLU	2.4
1	G	197	GLN	2.4
1	G	222	GLU	2.4
2	H	18	GLY	2.4
1	A	220	ASP	2.3

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.