Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 03:28 AM EDT

PDB ID	:	1TQ0
Title	:	Crystal structure of the potent anticoagulant thrombin mutant W215A/E217A in free form
Authors	:	Pineda, A.O.; Chen, Z.-W.; Caccia, S.; Savvides, S.N.; Waksman, G.; Mathews, F.S.; Di Cera, E.
Deposited on	:	2004-06-16
Resolution	:	2.80 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

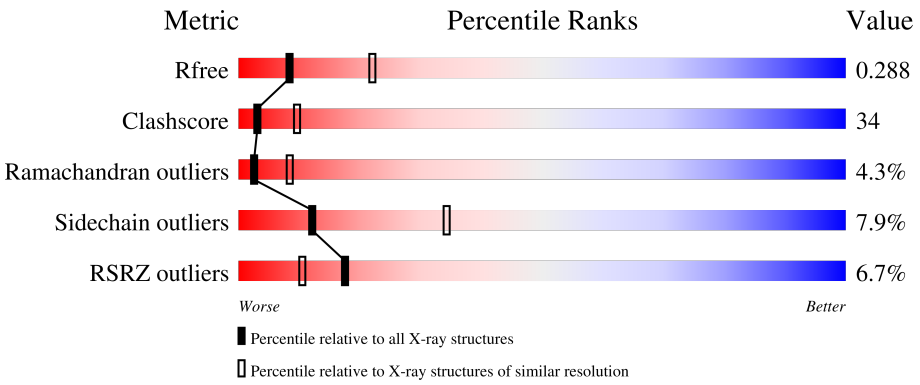
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	31	6%, 65%, 26%, 10%
1	C	31	58%, 29%, •, 10%
2	B	257	6%, 45%, 44%, 7%, •, •
2	D	257	7%, 44%, 44%, 8%, •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4637 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 Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	31	254	157	43	53	1	0	0	0
1	C	28	230	144	37	48	1	0	0	0

- Molecule 2 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	247	1992	1272	352	354	14	0	0	0
2	D	246	1985	1267	353	351	14	4	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	215	ALA	TRP	engineered mutation	UNP P00734
B	217	ALA	GLU	engineered mutation	UNP P00734
D	215	ALA	TRP	engineered mutation	UNP P00734
D	217	ALA	GLU	engineered mutation	UNP P00734

- Molecule 3 is water.

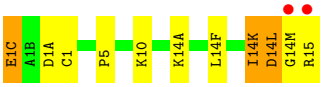
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	15	15	15	0	0
3	B	83	83	83	0	0
3	C	11	11	11	0	0
3	D	67	67	67	0	0

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.

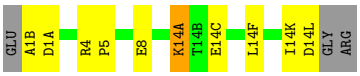
• Molecule 1: Prothrombin

Chain A:



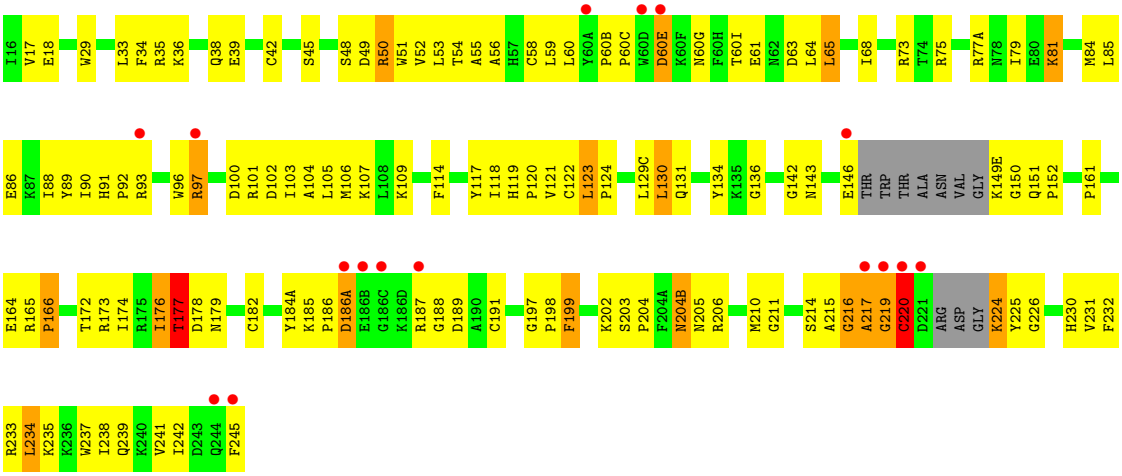
• Molecule 1: Prothrombin

Chain C:



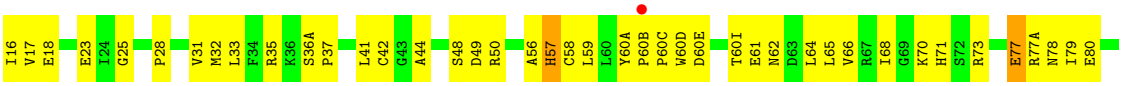
• Molecule 2: Prothrombin

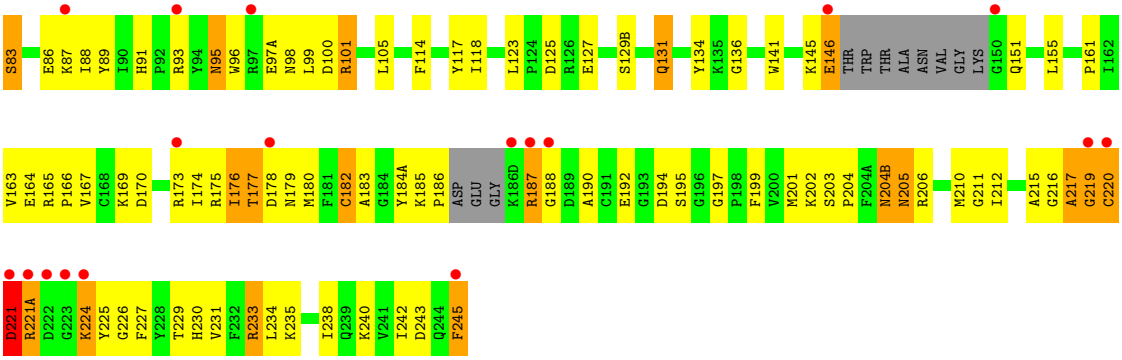
Chain B:



• Molecule 2: Prothrombin

Chain D:




S83
E86
K87
I88
Y89
I90
H91
P92
R93
Y94
N95
W96
R97
E97A
N98
L99
D100
R101
L105
F114
Y117
I118
L123
P124
D125
R126
E127
S129B
Q131
Y134
K135
G136
W141
K145
E146
THR
TRP
THR
ALA
ASN
VAL
GLY
LYS
G150
Q151
L155
P161
I162
V163
E164
R165
P166
V167
C168
K169
D170
R173
I174
R175
I176
T177
D178
N179
M180
F181
C182
A183
G184
Y184A
K185
P186
ASP
GLU
GLY
K186D
R187
G188
D189
A190
C191
E192
G193
D194
S195
G196
G197
P198
F199
V200
M201
K202
S203
P204
F204A
N204B
N205
R206
M210
G211
I212
A215
G216
A217
G219
C220
D221
R221A
D222
G223
K224
Y225
G226
F227
Y228
T229
H230
V231
F232
R233
L234
K235
I238
Q239
K240
V241
I242
D243
Q244
F245

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	131.93Å 131.93Å 131.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 15.03 – 2.81	Depositor EDS
% Data completeness (in resolution range)	91.7 (50.00-2.80) 93.6 (15.03-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.292 0.232 , 0.288	Depositor DCC
R_{free} test set	1202 reflections (6.54%)	wwPDB-VP
Wilson B-factor (Å^2)	76.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 68.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4637	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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	0.78	1/256 (0.4%)	0.94	0/340
1	C	0.62	0/232	0.88	1/309 (0.3%)
2	B	0.38	0/2041	0.69	2/2753 (0.1%)
2	D	0.34	0/2034	0.64	0/2744
All	All	0.41	1/4563 (0.0%)	0.69	3/6146 (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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14(M)	GLY	N-CA	7.18	1.56	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1(B)	ALA	CA-C-N	-6.15	103.67	117.20
2	B	220	CYS	N-CA-C	-5.77	95.42	111.00
2	B	199	PHE	N-CA-C	-5.37	96.51	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	117	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	254	0	251	7	0
1	C	230	0	229	7	0
2	B	1992	0	1980	150	0
2	D	1985	0	1974	153	0
3	A	15	0	0	0	0
3	B	83	0	0	1	0
3	C	11	0	0	0	0
3	D	67	0	0	3	0
All	All	4637	0	4434	301	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 34.

All (301) 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)
2:D:145:LYS:HG2	3:D:296:HOH:O	1.33	1.25
2:D:221(A):ARG:O	2:D:224:LYS:HE2	1.64	0.98
2:B:50:ARG:HH11	2:B:50:ARG:HB3	1.28	0.97
2:B:61:GLU:HG3	2:B:88:ILE:HG13	1.49	0.93
2:D:224:LYS:H	2:D:224:LYS:HD3	1.32	0.92
2:D:97(A):GLU:HG2	2:D:175:ARG:HH21	1.34	0.92
2:D:95:ASN:HD21	2:D:98:ASN:H	0.92	0.91
2:D:201:MET:SD	2:D:210:MET:HG3	2.10	0.91
2:B:107:LYS:HE3	2:B:245:PHE:HD2	1.36	0.90
2:D:95:ASN:ND2	2:D:98:ASN:H	1.73	0.86
2:B:149(E):LYS:HD3	2:D:173:ARG:HH22	1.41	0.86
2:B:173:ARG:HH11	2:D:35:ARG:HH22	1.24	0.85
2:D:73:ARG:NH1	2:D:151:GLN:HB3	1.91	0.85
2:B:105:LEU:HD13	2:B:242:ILE:HD11	1.59	0.84
2:D:177:THR:HG22	2:D:179:ASN:H	1.40	0.84
2:D:177:THR:CG2	2:D:179:ASN:H	1.93	0.81
2:B:176:ILE:H	2:B:176:ILE:CD1	1.92	0.81
2:D:211:GLY:HA2	2:D:231:VAL:HG23	1.61	0.80
2:D:233:ARG:HB3	2:D:233:ARG:NH1	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:97(A):GLU:HG2	2:D:175:ARG:NH2	1.97	0.79
2:D:95:ASN:HD21	2:D:98:ASN:N	1.77	0.79
2:D:146:GLU:HB3	2:D:220:CYS:HB3	1.66	0.77
2:B:149(E):LYS:HE3	2:B:151:GLN:CG	2.16	0.76
2:D:95:ASN:C	2:D:95:ASN:HD22	1.89	0.76
2:D:18:GLU:HG3	2:D:187:ARG:HG3	1.68	0.75
2:B:107:LYS:HE3	2:B:245:PHE:CD2	2.22	0.75
2:D:61:GLU:HG2	2:D:87:LYS:HA	1.68	0.74
2:D:17:VAL:HG12	2:D:18:GLU:HG2	1.70	0.73
2:B:189:ASP:OD1	2:B:217:ALA:HB3	1.89	0.72
2:D:100:ASP:OD1	2:D:177:THR:HG21	1.89	0.72
2:B:211:GLY:HA2	2:B:231:VAL:HG23	1.71	0.72
1:A:14(K):ILE:O	1:A:14(L):ASP:HB2	1.89	0.72
2:B:146:GLU:HB2	2:B:220:CYS:HB3	1.70	0.71
2:D:224:LYS:HD3	2:D:224:LYS:N	2.04	0.71
2:B:34:PHE:HB3	2:B:65:LEU:HD12	1.73	0.71
2:D:238:ILE:O	2:D:242:ILE:HG12	1.91	0.71
2:B:50:ARG:HB3	2:B:50:ARG:NH1	2.04	0.70
2:D:177:THR:HG23	2:D:178:ASP:N	2.06	0.70
2:B:149(E):LYS:CD	2:D:173:ARG:HH22	2.04	0.70
2:B:51:TRP:CD2	2:B:242:ILE:HD12	2.26	0.70
2:B:45:SER:HB3	2:B:198:PRO:HG3	1.73	0.70
2:B:176:ILE:H	2:B:176:ILE:HD12	1.55	0.69
2:B:149(E):LYS:HE3	2:B:151:GLN:HG3	1.74	0.69
2:B:217:ALA:HB2	2:B:226:GLY:N	2.07	0.69
2:B:18:GLU:HG3	2:B:187:ARG:CB	2.23	0.69
2:B:100:ASP:OD1	2:B:177:THR:HG21	1.94	0.68
2:D:95:ASN:ND2	2:D:95:ASN:C	2.47	0.68
2:D:61:GLU:HG3	2:D:88:ILE:HG13	1.74	0.68
2:D:73:ARG:HH12	2:D:151:GLN:HB3	1.59	0.68
2:D:60(I):THR:HG23	2:D:62:ASN:H	1.58	0.67
2:D:95:ASN:ND2	2:D:95:ASN:O	2.29	0.66
2:B:149(E):LYS:HA	2:D:173:ARG:NH1	2.10	0.66
2:D:215:ALA:HB3	2:D:227:PHE:HB2	1.79	0.65
2:B:61:GLU:HG3	2:B:88:ILE:CG1	2.25	0.64
2:B:18:GLU:HG3	2:B:187:ARG:HB2	1.79	0.64
2:B:232:PHE:C	2:B:234:LEU:H	2.01	0.64
2:D:169:LYS:O	2:D:169:LYS:HD3	1.98	0.64
2:B:73:ARG:CZ	2:B:151:GLN:HB3	2.28	0.64
2:B:185:LYS:O	2:B:186(A):ASP:N	2.24	0.64
2:B:149(E):LYS:HE3	2:B:151:GLN:HG2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ASP:CG	2:B:177:THR:HG21	2.19	0.63
2:B:237:TRP:O	2:B:241:VAL:HG23	1.98	0.63
2:B:35:ARG:HD3	2:B:39:GLU:OE1	1.98	0.63
2:B:177:THR:OG1	2:B:178:ASP:N	2.31	0.63
2:B:149(E):LYS:HG3	2:D:173:ARG:HH12	1.63	0.63
2:D:64:LEU:N	2:D:64:LEU:HD23	2.14	0.63
2:B:61:GLU:CG	2:B:88:ILE:HG13	2.27	0.63
2:D:230:HIS:ND1	2:D:233:ARG:HG3	2.14	0.62
2:B:149(E):LYS:HD3	2:D:173:ARG:NH2	2.12	0.62
2:B:216:GLY:O	2:B:219:GLY:N	2.33	0.62
1:C:14(C):GLU:OE1	2:D:202:LYS:HE2	2.01	0.61
2:D:177:THR:CG2	2:D:178:ASP:N	2.62	0.61
2:D:101:ARG:HE	2:D:179:ASN:ND2	1.98	0.61
2:D:176:ILE:HD13	2:D:176:ILE:H	1.65	0.61
1:C:14(K):ILE:O	1:C:14(K):ILE:HG22	2.00	0.61
1:C:14(C):GLU:HA	1:C:14(F):LEU:HD13	1.83	0.61
2:D:177:THR:HG22	2:D:179:ASN:N	2.15	0.60
2:D:217:ALA:HB1	2:D:224:LYS:HG2	1.84	0.60
2:B:238:ILE:O	2:B:242:ILE:HG12	2.00	0.60
2:B:136:GLY:HA3	2:B:199:PHE:CZ	2.37	0.60
2:B:93:ARG:NH2	2:B:101:ARG:HH21	1.99	0.60
2:B:60:LEU:HD23	2:B:60(B):PRO:HD3	1.83	0.59
2:B:149(E):LYS:CG	2:D:173:ARG:HH22	2.15	0.59
2:B:81:LYS:HE3	3:B:268:HOH:O	2.03	0.58
2:B:203:SER:HB3	2:B:204(B):ASN:ND2	2.19	0.58
2:D:177:THR:HG23	2:D:178:ASP:H	1.67	0.58
2:B:164:GLU:HB3	2:B:166:PRO:HD2	1.85	0.58
2:D:101:ARG:HH21	2:D:179:ASN:ND2	2.01	0.58
2:D:233:ARG:HB3	2:D:233:ARG:CZ	2.34	0.58
2:D:163:VAL:HG23	2:D:183:ALA:HA	1.86	0.57
2:B:174:ILE:HD12	2:B:174:ILE:N	2.19	0.57
2:D:33:LEU:HD23	2:D:42:CYS:HB2	1.85	0.56
2:B:203:SER:HB3	2:B:204(B):ASN:HD21	1.70	0.56
2:B:211:GLY:CA	2:B:231:VAL:HG23	2.35	0.56
2:D:16:ILE:N	2:D:194:ASP:OD2	2.38	0.56
2:D:177:THR:HG21	2:D:179:ASN:ND2	2.21	0.56
1:A:14(F):LEU:N	1:A:14(F):LEU:HD12	2.21	0.56
2:B:204(B):ASN:HD22	2:B:204(B):ASN:H	1.53	0.56
2:D:240:LYS:HD3	3:D:258:HOH:O	2.06	0.56
2:D:176:ILE:HG12	2:D:176:ILE:O	2.06	0.55
2:D:60(A):TYR:CD1	2:D:60(C):PRO:HD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1(C):GLU:H1	2:B:120:PRO:HG2	1.70	0.55
2:D:98:ASN:ND2	2:D:175:ARG:O	2.39	0.55
2:D:217:ALA:O	2:D:220:CYS:N	2.39	0.54
2:B:18:GLU:HG3	2:B:187:ARG:HB3	1.90	0.54
2:B:103:ILE:HG12	2:B:104:ALA:N	2.20	0.54
2:B:149(E):LYS:HG2	2:B:151:GLN:HG2	1.89	0.54
2:B:176:ILE:CD1	2:B:176:ILE:N	2.64	0.54
2:D:95:ASN:ND2	2:D:97(A):GLU:HB3	2.22	0.54
1:A:1:CYS:O	2:B:122:CYS:SG	2.65	0.54
2:B:93:ARG:NH2	2:B:101:ARG:NH2	2.56	0.54
2:D:176:ILE:HD13	2:D:176:ILE:N	2.22	0.54
2:D:91:HIS:CD2	2:D:101:ARG:HG2	2.43	0.54
2:B:59:LEU:HD13	2:B:88:ILE:HD13	1.90	0.54
2:B:34:PHE:HB3	2:B:65:LEU:CD1	2.37	0.54
2:D:211:GLY:CA	2:D:231:VAL:HG23	2.34	0.53
2:B:188:GLY:O	2:B:189:ASP:HB2	2.07	0.53
2:D:71:HIS:HB3	2:D:77:GLU:OE2	2.09	0.53
2:B:149(E):LYS:HB2	2:D:173:ARG:NH2	2.24	0.53
2:D:167:VAL:HG12	2:D:167:VAL:O	2.09	0.53
2:B:215:ALA:O	2:B:216:GLY:C	2.47	0.53
2:D:59:LEU:HD13	2:D:88:ILE:HD13	1.91	0.53
2:B:90:ILE:HG22	2:B:91:HIS:N	2.24	0.53
2:B:60(I):THR:HG22	2:B:63:ASP:OD2	2.09	0.52
2:B:50:ARG:NH1	2:B:107:LYS:NZ	2.58	0.52
2:B:86:GLU:HB2	2:B:109:LYS:HA	1.90	0.52
2:B:17:VAL:HG23	2:B:191:CYS:HB2	1.92	0.52
2:B:50:ARG:HH11	2:B:50:ARG:CB	2.12	0.52
2:D:56:ALA:C	2:D:58:CYS:H	2.13	0.52
2:B:143:ASN:HA	2:B:150:GLY:O	2.10	0.52
2:B:96:TRP:CZ3	2:B:97:ARG:HG2	2.45	0.52
2:B:149(E):LYS:CG	2:B:150:GLY:N	2.72	0.52
2:B:36:LYS:HZ3	2:B:84:MET:HE2	1.76	0.51
2:B:176:ILE:O	2:B:177:THR:O	2.28	0.51
2:D:78:ASN:C	2:D:79:ILE:HD13	2.29	0.51
2:B:224:LYS:NZ	2:B:224:LYS:HB3	2.25	0.51
2:D:169:LYS:HG2	2:D:176:ILE:CD1	2.41	0.51
2:B:85:LEU:HD22	2:B:106:MET:HB3	1.93	0.51
2:D:33:LEU:CD2	2:D:42:CYS:HB2	2.41	0.51
2:D:176:ILE:HG22	2:D:227:PHE:CE2	2.46	0.51
2:D:221(A):ARG:O	2:D:224:LYS:CE	2.48	0.51
2:B:149(E):LYS:CG	2:B:150:GLY:H	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:TRP:CE2	2:B:242:ILE:HD12	2.45	0.51
2:D:230:HIS:CE1	2:D:233:ARG:HG3	2.45	0.51
2:D:169:LYS:HD3	2:D:169:LYS:C	2.31	0.50
2:B:119:HIS:CD2	2:B:120:PRO:HD2	2.47	0.50
2:D:164:GLU:HB3	2:D:166:PRO:HD2	1.93	0.50
2:D:204(B):ASN:HD22	2:D:204(B):ASN:C	2.14	0.50
2:B:59:LEU:HD22	2:B:64:LEU:HD11	1.92	0.50
2:B:59:LEU:HB2	2:B:90:ILE:HD11	1.93	0.50
2:B:235:LYS:HE2	2:B:239:GLN:NE2	2.26	0.50
2:D:243:ASP:C	2:D:245:PHE:H	2.14	0.50
2:D:31:VAL:HB	2:D:44:ALA:HB3	1.93	0.49
2:D:56:ALA:O	2:D:58:CYS:N	2.45	0.49
2:D:176:ILE:H	2:D:176:ILE:CD1	2.24	0.49
2:B:36:LYS:NZ	2:B:84:MET:HE2	2.27	0.49
2:B:77(A):ARG:O	2:B:79:ILE:HG12	2.11	0.49
2:B:149(E):LYS:HA	2:D:173:ARG:HH12	1.78	0.49
2:D:217:ALA:HB2	2:D:226:GLY:N	2.27	0.49
2:D:217:ALA:HB2	2:D:225:TYR:C	2.32	0.49
2:D:177:THR:H	2:D:180:MET:HE3	1.77	0.49
2:D:203:SER:HB3	2:D:204(B):ASN:HD21	1.77	0.49
2:B:204(B):ASN:OD1	2:B:206:ARG:HD2	2.13	0.49
2:B:161:PRO:HD3	2:B:184(A):TYR:CZ	2.47	0.49
2:D:145:LYS:O	2:D:146:GLU:HB2	2.13	0.48
2:D:187:ARG:HH11	2:D:187:ARG:HG2	1.78	0.48
2:B:102:ASP:OD2	2:B:214:SER:OG	2.27	0.48
2:B:185:LYS:C	2:B:186(A):ASP:H	2.13	0.48
2:D:233:ARG:HB3	2:D:233:ARG:HH11	1.72	0.48
2:B:35:ARG:O	2:B:38:GLN:HA	2.13	0.48
2:B:65:LEU:HD12	2:B:65:LEU:O	2.13	0.48
2:B:232:PHE:C	2:B:234:LEU:N	2.67	0.48
2:B:104:ALA:HA	2:B:237:TRP:HH2	1.79	0.48
2:B:165:ARG:N	2:B:166:PRO:CD	2.77	0.48
2:D:243:ASP:C	2:D:245:PHE:N	2.66	0.48
1:A:1(C):GLU:N	2:B:120:PRO:HG2	2.28	0.48
2:B:149(E):LYS:HB2	2:D:173:ARG:HH22	1.79	0.48
2:D:78:ASN:O	2:D:79:ILE:HD13	2.13	0.48
2:B:101:ARG:HG3	2:B:101:ARG:NH1	2.28	0.47
2:D:57:HIS:HB3	2:D:99:LEU:HD22	1.97	0.47
2:D:190:ALA:O	2:D:216:GLY:HA3	2.14	0.47
2:B:51:TRP:CZ2	2:B:107:LYS:HE2	2.50	0.47
2:B:60(C):PRO:HD3	2:B:96:TRP:CE3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129(C):LEU:O	2:B:134:TYR:HD2	1.98	0.47
2:D:41:LEU:CD1	2:D:64:LEU:HD13	2.45	0.47
1:C:14(F):LEU:N	1:C:14(F):LEU:HD12	2.30	0.47
2:D:77(A):ARG:O	2:D:78:ASN:HB2	2.13	0.47
2:D:204(B):ASN:ND2	2:D:206:ARG:H	2.12	0.47
2:D:146:GLU:OE2	2:D:221(A):ARG:HB2	2.15	0.47
2:B:149(E):LYS:HG2	2:B:150:GLY:N	2.31	0.46
2:D:60(D):TRP:O	2:D:60(E):ASP:HB2	2.15	0.46
2:B:60(B):PRO:HD2	2:B:96:TRP:CG	2.50	0.46
2:B:60(E):ASP:OD2	2:B:60(E):ASP:N	2.47	0.46
2:D:61:GLU:N	2:D:61:GLU:OE1	2.49	0.46
2:B:101:ARG:HG3	2:B:101:ARG:HH11	1.81	0.46
2:D:146:GLU:CB	2:D:220:CYS:HB3	2.41	0.46
2:B:185:LYS:HG2	2:B:225:TYR:OH	2.16	0.46
2:B:114:PHE:CZ	2:B:120:PRO:HG3	2.50	0.46
2:D:57:HIS:HB3	2:D:99:LEU:CD2	2.46	0.46
2:D:131:GLN:O	2:D:134:TYR:HB2	2.15	0.46
2:D:161:PRO:HG3	2:D:184(A):TYR:CD1	2.51	0.46
2:D:221:ASP:O	2:D:221(A):ARG:C	2.54	0.46
2:B:232:PHE:O	2:B:234:LEU:N	2.46	0.45
2:B:45:SER:O	2:B:52:VAL:HA	2.16	0.45
2:B:49:ASP:OD1	2:B:50:ARG:HG3	2.16	0.45
2:B:172:THR:OG1	2:B:174:ILE:HD13	2.16	0.45
1:C:14(A):LYS:HB2	2:D:23:GLU:OE2	2.17	0.45
2:B:177:THR:OG1	2:B:179:ASN:ND2	2.50	0.45
2:D:70:LYS:HG2	2:D:80:GLU:HB3	1.99	0.45
2:B:73:ARG:NH1	2:B:152:PRO:O	2.47	0.45
2:D:25:GLY:O	2:D:28:PRO:HD3	2.16	0.45
2:D:105:LEU:HD13	2:D:242:ILE:HD11	1.99	0.45
2:D:136:GLY:HA3	2:D:199:PHE:CZ	2.52	0.45
2:B:48:SER:HG	2:B:51:TRP:HD1	1.65	0.45
2:B:60(B):PRO:HG2	2:B:96:TRP:CE2	2.52	0.44
2:D:33:LEU:HB3	2:D:42:CYS:H	1.82	0.44
2:B:91:HIS:CE1	2:B:101:ARG:HD3	2.52	0.44
2:D:49:ASP:HB3	2:D:114:PHE:CZ	2.53	0.44
2:B:56:ALA:C	2:B:58:CYS:H	2.19	0.44
2:D:141:TRP:CZ2	2:D:155:LEU:HD13	2.53	0.44
2:B:53:LEU:HD11	2:B:103:ILE:HD11	2.00	0.44
2:D:88:ILE:HG22	2:D:89:TYR:N	2.33	0.44
2:B:33:LEU:HD21	2:B:59:LEU:HD21	1.98	0.44
1:A:5:PRO:O	1:A:10:LYS:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:HIS:HA	2:B:237:TRP:CZ2	2.52	0.43
2:D:169:LYS:HG2	2:D:176:ILE:HD11	1.99	0.43
2:B:45:SER:HB3	2:B:198:PRO:CG	2.46	0.43
2:B:65:LEU:HD12	2:B:65:LEU:C	2.38	0.43
2:B:189:ASP:OD1	2:B:217:ALA:CB	2.64	0.43
2:D:93:ARG:NE	2:D:101:ARG:HH11	2.16	0.43
2:D:145:LYS:NZ	3:D:310:HOH:O	2.51	0.43
2:D:125:ASP:OD2	2:D:127:GLU:HB2	2.18	0.43
2:B:203:SER:HA	2:B:204:PRO:HD3	1.91	0.43
2:D:36(A):SER:HA	2:D:37:PRO:C	2.39	0.43
2:D:68:ILE:O	2:D:80:GLU:HA	2.18	0.43
2:D:165:ARG:N	2:D:166:PRO:CD	2.82	0.43
2:D:203:SER:HB3	2:D:204(B):ASN:ND2	2.33	0.43
2:D:169:LYS:CG	2:D:176:ILE:HD11	2.48	0.43
2:B:36:LYS:NZ	2:B:84:MET:CE	2.82	0.43
2:D:235:LYS:HA	2:D:238:ILE:HD12	1.99	0.43
2:B:217:ALA:O	2:B:219:GLY:C	2.56	0.43
2:D:101:ARG:NH2	2:D:179:ASN:ND2	2.67	0.43
2:D:31:VAL:HG12	2:D:32:MET:N	2.34	0.43
2:D:177:THR:HG21	2:D:179:ASN:HD22	1.83	0.43
2:D:204(B):ASN:HD22	2:D:205:ASN:N	2.17	0.43
2:B:29:TRP:CG	2:B:121:VAL:HB	2.54	0.42
2:D:64:LEU:N	2:D:64:LEU:CD2	2.80	0.42
2:D:174:ILE:HG22	2:D:175:ARG:N	2.34	0.42
2:B:124:PRO:HG3	2:B:210:MET:SD	2.59	0.42
2:B:164:GLU:CB	2:B:166:PRO:HD2	2.48	0.42
2:D:101:ARG:NE	2:D:179:ASN:ND2	2.65	0.42
2:D:117:TYR:C	2:D:118:ILE:HG13	2.39	0.42
2:B:149(E):LYS:CB	2:D:173:ARG:HH22	2.32	0.42
2:D:212:ILE:HB	2:D:229:THR:HB	2.02	0.42
2:B:123:LEU:HD12	2:B:123:LEU:HA	1.78	0.42
2:B:88:ILE:HG22	2:B:89:TYR:N	2.35	0.42
2:D:66:VAL:HG23	2:D:83:SER:HB3	2.02	0.42
2:B:90:ILE:CG2	2:B:91:HIS:N	2.83	0.42
2:B:202:LYS:NZ	2:B:205:ASN:O	2.53	0.42
2:D:95:ASN:CG	2:D:97(A):GLU:HB3	2.40	0.42
2:B:50:ARG:NH1	2:B:107:LYS:HZ2	2.18	0.42
2:B:54:THR:HG23	2:B:55:ALA:O	2.20	0.42
2:B:68:ILE:HG22	2:B:118:ILE:HG12	2.02	0.42
2:B:176:ILE:N	2:B:176:ILE:HD13	2.34	0.42
2:D:93:ARG:NE	2:D:101:ARG:NH1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:221(A):ARG:HB3	2:D:224:LYS:HE2	2.02	0.42
1:A:14(F):LEU:N	1:A:14(F):LEU:CD1	2.83	0.41
2:B:186(A):ASP:N	2:B:186(A):ASP:OD1	2.53	0.41
1:C:4:ARG:HB2	1:C:8:GLU:OE1	2.19	0.41
2:D:182:CYS:HA	2:D:226:GLY:O	2.19	0.41
2:B:60(B):PRO:HD2	2:B:96:TRP:CD2	2.55	0.41
2:B:121:VAL:HG22	2:B:122:CYS:H	1.85	0.41
2:D:17:VAL:O	2:D:188:GLY:HA2	2.20	0.41
2:B:33:LEU:HB3	2:B:42:CYS:H	1.85	0.41
2:B:91:HIS:ND1	2:B:92:PRO:HD2	2.35	0.41
2:D:60(B):PRO:O	2:D:60(D):TRP:N	2.53	0.41
2:D:60(C):PRO:C	2:D:60(D):TRP:HD1	2.23	0.41
2:B:75:ARG:HG3	2:B:75:ARG:HH11	1.85	0.41
2:B:130:LEU:HD13	2:B:230:HIS:NE2	2.35	0.41
2:D:146:GLU:CD	2:D:221(A):ARG:HH21	2.24	0.41
2:D:185:LYS:HA	2:D:186:PRO:HD3	1.92	0.41
2:D:60(C):PRO:HD3	2:D:96:TRP:CZ3	2.55	0.41
2:D:100:ASP:OD2	2:D:101:ARG:NH2	2.54	0.41
2:B:100:ASP:O	2:B:101:ARG:HB2	2.21	0.41
2:B:142:GLY:O	2:B:152:PRO:HD3	2.20	0.41
2:B:217:ALA:HB2	2:B:225:TYR:C	2.40	0.41
2:D:48:SER:OG	2:D:49:ASP:N	2.53	0.41
2:D:216:GLY:O	2:D:219:GLY:N	2.54	0.41
2:B:217:ALA:O	2:B:220:CYS:N	2.54	0.41
2:D:101:ARG:NH2	2:D:179:ASN:HD21	2.19	0.41
2:B:197:GLY:HA2	2:B:198:PRO:HD3	1.92	0.40
2:D:177:THR:HG23	2:D:179:ASN:H	1.82	0.40
2:B:50:ARG:NH1	2:B:107:LYS:HZ3	2.20	0.40
2:B:60:LEU:HD23	2:B:60:LEU:C	2.42	0.40
2:B:131:GLN:O	2:B:134:TYR:HB2	2.21	0.40
1:C:4:ARG:HA	1:C:5:PRO:HD3	1.94	0.40
2:D:33:LEU:HD12	2:D:33:LEU:HA	1.94	0.40
2:D:101:ARG:HG3	2:D:234:LEU:HD21	2.04	0.40
2:D:169:LYS:CB	2:D:176:ILE:HD11	2.52	0.40
2:D:195:SER:C	2:D:197:GLY:H	2.23	0.40
2:D:203:SER:HA	2:D:204:PRO:HD3	1.98	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	29/31 (94%)	24 (83%)	1 (3%)	4 (14%)	0 0
1	C	26/31 (84%)	20 (77%)	5 (19%)	1 (4%)	3 10
2	B	241/257 (94%)	205 (85%)	25 (10%)	11 (5%)	2 7
2	D	240/257 (93%)	203 (85%)	30 (12%)	7 (3%)	4 15
All	All	536/576 (93%)	452 (84%)	61 (11%)	23 (4%)	2 8

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14(L)	ASP
2	B	177	THR
2	B	217	ALA
2	D	217	ALA
2	D	220	CYS
1	A	14(A)	LYS
2	B	186	PRO
2	B	216	GLY
2	D	57	HIS
2	D	77	GLU
2	D	219	GLY
2	D	221	ASP
1	A	1(A)	ASP
1	A	14(K)	ILE
2	B	220	CYS
2	B	60(G)	ASN
2	B	166	PRO
2	B	219	GLY
2	B	233	ARG
1	C	14(A)	LYS
2	B	130	LEU
2	B	234	LEU
2	D	221(A)	ARG

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	28/28 (100%)	26 (93%)	2 (7%)	14	39
1	C	26/28 (93%)	24 (92%)	2 (8%)	13	35
2	B	215/222 (97%)	203 (94%)	12 (6%)	21	51
2	D	214/222 (96%)	192 (90%)	22 (10%)	7	21
All	All	483/500 (97%)	445 (92%)	38 (8%)	12	34

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1(C)	GLU
1	A	15	ARG
2	B	50	ARG
2	B	60(E)	ASP
2	B	65	LEU
2	B	81	LYS
2	B	97	ARG
2	B	123	LEU
2	B	176	ILE
2	B	177	THR
2	B	182	CYS
2	B	186(A)	ASP
2	B	204(B)	ASN
2	B	224	LYS
1	C	1(A)	ASP
1	C	14(L)	ASP
2	D	50	ARG
2	D	65	LEU
2	D	83	SER
2	D	86	GLU
2	D	95	ASN
2	D	101	ARG
2	D	123	LEU
2	D	129(B)	SER

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Mol	Chain	Res	Type
2	D	131	GLN
2	D	146	GLU
2	D	170	ASP
2	D	176	ILE
2	D	177	THR
2	D	182	CYS
2	D	187	ARG
2	D	192	GLU
2	D	204(B)	ASN
2	D	205	ASN
2	D	221	ASP
2	D	224	LYS
2	D	233	ARG
2	D	245	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	38	GLN
2	B	71	HIS
2	B	143	ASN
2	B	179	ASN
2	B	204(B)	ASN
2	B	205	ASN
2	B	209	GLN
2	B	239	GLN
2	D	60(G)	ASN
2	D	95	ASN
2	D	156	GLN
2	D	179	ASN
2	D	204(B)	ASN
2	D	209	GLN
2	D	239	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	31/31 (100%)	-0.04	2 (6%) 18 11	39, 61, 90, 99	0
1	C	28/31 (90%)	-0.18	0 100 100	48, 61, 78, 92	0
2	B	247/257 (96%)	0.08	16 (6%) 18 11	40, 71, 99, 99	0
2	D	246/257 (95%)	0.13	19 (7%) 13 7	44, 74, 99, 99	2 (0%)
All	All	552/576 (95%)	0.08	37 (6%) 17 10	39, 72, 99, 99	2 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	221	ASP	6.8
2	D	223	GLY	6.7
2	D	219	GLY	4.9
2	D	221(A)	ARG	4.7
2	D	222	ASP	4.3
2	B	245	PHE	4.3
2	B	220	CYS	4.1
1	A	14(M)	GLY	4.0
2	B	186(C)	GLY	4.0
2	B	186(A)	ASP	3.4
2	D	173	ARG	3.3
2	D	150	GLY	3.2
2	B	221	ASP	3.1
2	B	219	GLY	2.9
2	D	178	ASP	2.9
2	D	220	CYS	2.8
2	B	217	ALA	2.8
1	A	15	ARG	2.7
2	B	60(E)	ASP	2.7
2	D	245	PHE	2.5
2	B	244	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	186(D)	LYS	2.4
2	B	60(D)	TRP	2.4
2	B	146	GLU	2.4
2	D	188	GLY	2.3
2	D	187	ARG	2.3
2	D	146	GLU	2.3
2	B	93	ARG	2.3
2	B	186(B)	GLU	2.3
2	D	93	ARG	2.2
2	D	224	LYS	2.1
2	B	187	ARG	2.1
2	D	97	ARG	2.1
2	D	60(B)	PRO	2.1
2	B	97	ARG	2.1
2	B	60(A)	TYR	2.1
2	D	87	LYS	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.