



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:48 am BST

PDB ID : 2UZK
Title : Crystal structure of the human FOXO3a-DBD bound to DNA
Authors : Tsai, K.-L.; Sun, Y.-J.; Huang, C.-Y.; Yang, J.-Y.; Hung, M.-C.; Hsiao, C.-D.
Deposited on : 2007-04-30
Resolution : 2.70 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

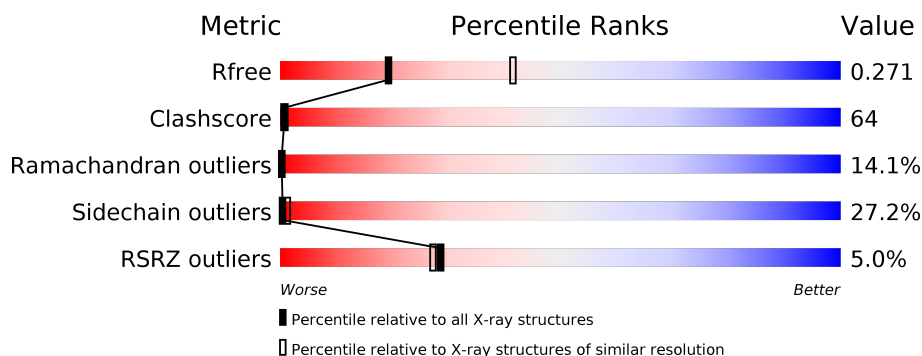
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	97	<div> <div>9%</div> <div>28% 44% 19% 9%</div> </div>
1	C	97	<div> <div>3%</div> <div>15% 52% 24% 5%</div> </div>
2	B	13	<div> <div>8%</div> <div>85% 8%</div> </div>
2	D	13	<div> <div>15%</div> <div>85%</div> </div>
3	E	13	<div> <div>8%</div> <div>85% 8%</div> </div>
3	F	13	<div> <div>8%</div> <div>92%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2741 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 FORKHEAD BOX PROTEIN O3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	97	Total	C	N	O	S	0	0	0
			774	481	147	142	4			
1	C	92	Total	C	N	O	S	0	0	1
			704	437	131	133	3			

- Molecule 2 is a DNA chain called 5'-D(*CP*TP*AP*TP*GP*TP*AP*AP*AP*CP*AP*A P*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	P	0	0	0
			262	127	50	73	12			
2	D	13	Total	C	N	O	P	0	0	0
			262	127	50	73	12			

- Molecule 3 is a DNA chain called 5'-D(*GP*TP*TP*GP*TP*TP*TP*AP*CP*AP*TP*AP *G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	13	Total	C	N	O	P	0	0	0
			265	129	45	79	12			
3	F	13	Total	C	N	O	P	0	0	0
			265	129	45	79	12			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total	O	0	0
			46	46		
4	B	15	Total	O	0	0
			15	15		
4	C	72	Total	O	0	0
			72	72		

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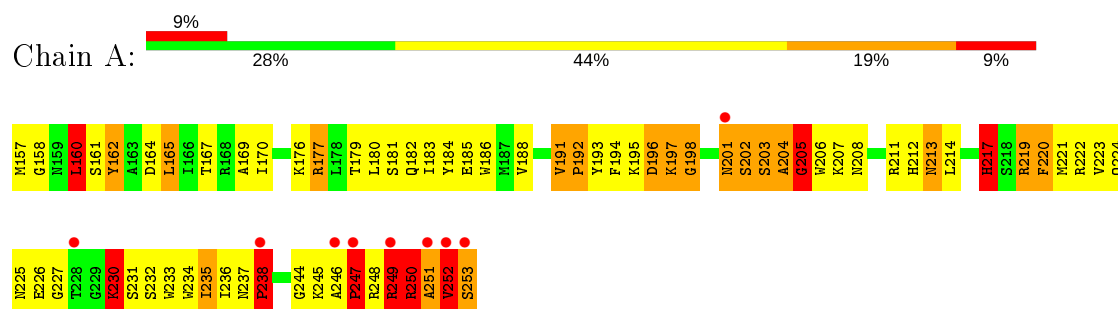
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	33	Total 33	O 33	0	0
4	E	22	Total 22	O 22	0	0
4	F	21	Total 21	O 21	0	0

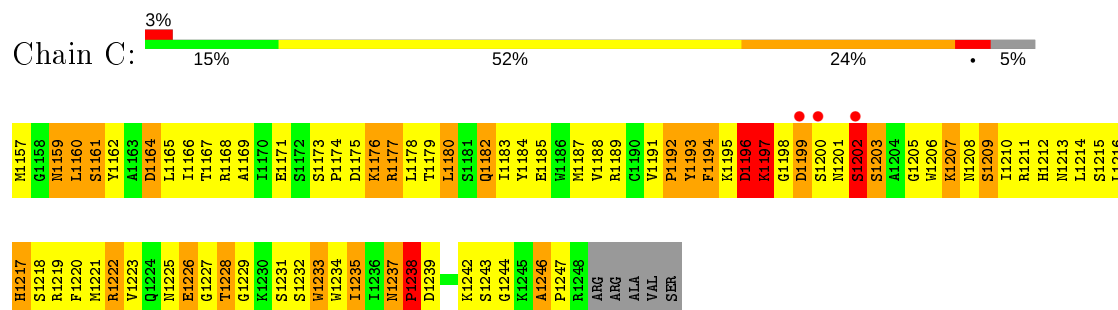
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: FORKHEAD BOX PROTEIN O3A



• Molecule 1: FORKHEAD BOX PROTEIN O3A



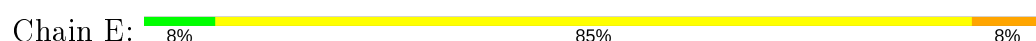
• Molecule 2: 5'-D(*CP*TP*AP*TP*GP*TP*AP*AP*AP*CP*AP*AP*C)-3'



• Molecule 2: 5'-D(*CP*TP*AP*TP*GP*TP*AP*AP*AP*CP*AP*AP*C)-3'



• Molecule 3: 5'-D(*GP*TP*TP*GP*TP*TP*TP*AP*CP*AP*TP*AP*G)-3'



G25	T26	T27	G28	T29	T30	T31	A32	C33	A34	T35	A36	G37
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● Molecule 3: 5'-D(*GP*TP*TP*GP*TP*TP*TP*AP*CP*AP*TP*AP*G)-3'



G1025	T1026	T1027	G1028	T1029	T1030	T1031	A1032	C1033	A1034	T1035	A1036	G1037
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4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	41.96 Å 41.96 Å 354.82 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.13 – 2.70 24.12 – 2.61	Depositor EDS
% Data completeness (in resolution range)	94.6 (24.13-2.70) 92.2 (24.12-2.61)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.84 (at 2.60 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.266 0.240 , 0.271	Depositor DCC
R_{free} test set	495 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , 106.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.26$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.399 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	2741	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.75	2/792 (0.3%)	1.22	15/1064 (1.4%)
1	C	0.63	1/721 (0.1%)	1.50	10/972 (1.0%)
2	B	0.98	3/294 (1.0%)	1.20	6/451 (1.3%)
2	D	0.59	0/294	0.79	0/451
3	E	0.78	1/296 (0.3%)	0.87	0/456
3	F	0.49	0/296	0.83	0/456
All	All	0.71	7/2693 (0.3%)	1.18	31/3850 (0.8%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	DC	O3'-P	10.65	1.74	1.61
3	E	37	DG	P-O5'	-8.27	1.51	1.59
1	C	1203	SER	CA-CB	7.60	1.64	1.52
1	A	247	PRO	C-N	-7.59	1.16	1.34
1	A	245	LYS	CB-CG	6.80	1.71	1.52
2	B	2	DT	O3'-P	-6.16	1.53	1.61
2	B	2	DT	C3'-O3'	-5.33	1.37	1.44

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1237	ASN	C-N-CD	-21.96	72.29	120.60
1	C	1237	ASN	C-N-CA	12.43	174.22	122.00
1	C	1202	SER	C-N-CA	11.24	149.79	121.70
2	B	2	DT	O5'-P-OP1	-10.15	96.57	105.70
1	C	1196	ASP	N-CA-C	9.49	136.63	111.00
1	C	1197	LYS	N-CA-C	7.84	132.16	111.00
1	A	245	LYS	CD-CE-NZ	7.79	129.61	111.70
1	A	252	VAL	CA-CB-CG1	-7.58	99.53	110.90
2	B	1	DC	P-O3'-C3'	7.47	128.67	119.70
1	A	251	ALA	N-CA-C	-7.23	91.48	111.00
1	A	202	SER	N-CA-C	6.82	129.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1203	SER	N-CA-CB	-6.68	100.48	110.50
2	B	1	DC	OP1-P-O3'	6.59	119.69	105.20
1	C	1161	SER	N-CA-C	6.51	128.57	111.00
1	A	230	LYS	N-CA-C	6.47	128.48	111.00
1	A	205	GLY	N-CA-C	6.43	129.18	113.10
1	A	201	ASN	N-CA-C	6.42	128.32	111.00
1	A	252	VAL	CA-CB-CG2	6.23	120.24	110.90
1	A	160	LEU	N-CA-C	5.91	126.96	111.00
2	B	2	DT	O5'-P-OP2	5.87	117.74	110.70
1	C	1199	ASP	N-CA-C	5.81	126.68	111.00
1	C	1202	SER	O-C-N	-5.77	113.47	122.70
2	B	3	DA	O5'-P-OP2	-5.74	100.54	105.70
1	A	249	ARG	N-CA-C	5.61	126.15	111.00
1	A	253	SER	N-CA-C	5.47	125.76	111.00
1	A	252	VAL	N-CA-CB	5.45	123.50	111.50
1	A	196	ASP	N-CA-C	5.32	125.37	111.00
1	C	1202	SER	N-CA-CB	-5.23	102.65	110.50
2	B	3	DA	P-O5'-C5'	5.11	129.08	120.90
1	A	252	VAL	C-N-CA	5.08	134.40	121.70
1	A	252	VAL	O-C-N	5.00	130.70	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	774	0	764	101	0
1	C	704	0	659	100	0
2	B	262	0	148	24	0
2	D	262	0	148	29	0
3	E	265	0	151	26	0
3	F	265	0	151	37	0
4	A	46	0	0	3	0
4	B	15	0	0	0	0
4	C	72	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	33	0	0	0	0
4	E	22	0	0	0	0
4	F	21	0	0	0	0
All	All	2741	0	2021	285	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 64.

All (285) 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:1007:DA:H2''	2:D:1008:DA:H5'	1.26	1.14
1:C:1237:ASN:ND2	1:C:1238:PRO:HD3	1.68	1.07
1:A:237:ASN:HB2	1:A:238:PRO:HD2	1.11	1.05
1:A:160:LEU:HD12	1:A:165:LEU:HD22	1.39	1.05
2:B:5:DG:H2''	2:B:6:DT:H5''	1.37	1.03
1:A:196:ASP:O	1:A:201:ASN:HA	1.58	1.03
3:F:1028:DG:H2''	3:F:1029:DT:H5''	1.06	1.03
1:A:251:ALA:O	1:A:252:VAL:CG2	2.07	1.01
3:F:1028:DG:C2'	3:F:1029:DT:H5''	1.91	1.00
3:F:1029:DT:H2''	3:F:1030:DT:H5'	1.50	0.94
3:F:1033:DC:H1'	3:F:1034:DA:C8	2.03	0.92
1:A:237:ASN:CB	1:A:238:PRO:HD2	1.99	0.92
3:F:1028:DG:H2''	3:F:1029:DT:C5'	1.97	0.92
1:A:188:VAL:HG11	1:A:198:GLY:N	1.86	0.90
1:A:177:ARG:HB2	1:A:233:TRP:HB3	1.53	0.89
1:A:213:ASN:HD22	1:A:213:ASN:H	1.16	0.89
1:C:1177:ARG:HH21	1:C:1177:ARG:CG	1.85	0.88
1:A:188:VAL:HG11	1:A:198:GLY:H	1.37	0.88
1:A:251:ALA:O	1:A:252:VAL:HG23	1.73	0.88
3:E:35:DT:H2''	3:E:36:DA:C8	2.09	0.88
2:D:1006:DT:H3	3:F:1032:DA:H61	1.19	0.86
3:F:1032:DA:H2''	3:F:1033:DC:O5'	1.75	0.85
2:B:9:DA:H2''	2:B:10:DC:O5'	1.76	0.85
3:F:1033:DC:OP2	3:F:1033:DC:H3'	1.75	0.85
2:D:1007:DA:C2'	2:D:1008:DA:H5'	2.07	0.85
1:A:237:ASN:HB2	1:A:238:PRO:CD	2.03	0.85
1:A:196:ASP:CG	1:A:203:SER:HB2	1.97	0.85
1:A:170:ILE:HD11	1:A:234:TRP:O	1.77	0.84
1:A:251:ALA:O	1:A:252:VAL:HG22	1.77	0.84
1:C:1177:ARG:HG3	1:C:1177:ARG:HH21	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1030:DT:H1'	3:F:1031:DT:H5''	1.60	0.84
1:A:226:GLU:OE2	1:C:1222:ARG:NE	2.10	0.84
1:A:176:LYS:HD2	1:C:1175:ASP:CG	1.99	0.82
1:A:185:GLU:OE2	1:A:197:LYS:HE2	1.80	0.82
1:A:196:ASP:OD1	1:A:203:SER:HB2	1.80	0.81
1:A:160:LEU:CD1	1:A:165:LEU:HD22	2.11	0.81
1:A:224:GLN:OE1	1:A:232:SER:HB2	1.79	0.80
1:A:196:ASP:OD2	1:A:206:TRP:NE1	2.15	0.80
2:D:1006:DT:H3	3:F:1032:DA:N6	1.80	0.80
3:E:35:DT:OP1	3:E:35:DT:H4'	1.81	0.79
1:C:1221:MET:SD	1:C:1235:ILE:HD11	2.23	0.79
1:C:1221:MET:HG2	1:C:1222:ARG:N	1.99	0.77
2:D:1009:DA:H2'	2:D:1010:DC:C6	2.19	0.77
2:D:1005:DG:H2''	2:D:1006:DT:O5'	1.83	0.77
1:A:224:GLN:HA	1:A:231:SER:O	1.85	0.77
2:D:1002:DT:H2''	2:D:1003:DA:H8	1.50	0.76
3:F:1035:DT:H2''	3:F:1036:DA:O5'	1.84	0.76
1:A:180:LEU:HB3	1:A:184:TYR:CE2	2.21	0.75
1:A:246:ALA:O	1:A:248:ARG:HD2	1.87	0.75
1:C:1179:THR:OG1	1:C:1182:GLN:HG2	1.87	0.75
3:F:1033:DC:H4'	3:F:1034:DA:O5'	1.87	0.75
2:D:1009:DA:H2''	2:D:1010:DC:O5'	1.87	0.74
1:A:160:LEU:HD12	1:A:165:LEU:CD2	2.15	0.74
1:A:176:LYS:CE	1:A:236:ILE:H	2.00	0.74
3:F:1032:DA:C2'	3:F:1033:DC:H2'	2.18	0.74
1:A:213:ASN:HD22	1:A:213:ASN:N	1.84	0.74
2:B:5:DG:C2'	2:B:6:DT:H5''	2.15	0.74
1:A:176:LYS:HE2	1:A:236:ILE:H	1.52	0.73
1:C:1175:ASP:C	1:C:1176:LYS:HG2	2.09	0.73
3:E:28:DG:H1'	3:E:29:DT:H5''	1.69	0.73
1:A:230:LYS:O	1:A:230:LYS:HG3	1.89	0.73
1:A:188:VAL:CG1	1:A:198:GLY:H	2.00	0.72
2:B:11:DA:H2''	2:B:12:DA:C5'	2.19	0.72
3:F:1029:DT:H2'	3:F:1030:DT:H71	1.70	0.72
3:F:1032:DA:H2''	3:F:1033:DC:H2'	1.73	0.71
1:A:176:LYS:HZ1	1:A:236:ILE:HB	1.55	0.71
1:A:212:HIS:HD2	3:E:30:DT:O4	1.73	0.71
1:C:1198:GLY:O	1:C:1199:ASP:HB3	1.90	0.71
1:A:181:SER:O	1:A:185:GLU:HG2	1.91	0.71
1:C:1225:ASN:O	1:C:1229:GLY:HA3	1.91	0.71
2:B:12:DA:H2''	2:B:13:DC:O5'	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ARG:O	1:A:236:ILE:HA	1.92	0.70
2:B:5:DG:H2"	2:B:6:DT:C5'	2.18	0.70
1:A:246:ALA:HB3	1:A:248:ARG:HH11	1.57	0.69
2:B:11:DA:H2"	2:B:12:DA:H5"	1.75	0.69
1:C:1161:SER:OG	2:D:1005:DG:P	2.51	0.69
2:D:1009:DA:H4'	2:D:1009:DA:OP1	1.93	0.69
1:C:1177:ARG:CG	1:C:1177:ARG:NH2	2.52	0.68
1:C:1185:GLU:O	1:C:1188:VAL:HG22	1.92	0.68
2:D:1002:DT:H2"	2:D:1003:DA:C8	2.29	0.68
3:F:1030:DT:C1'	3:F:1031:DT:H5"	2.24	0.68
1:C:1207:LYS:HB3	1:C:1207:LYS:NZ	2.08	0.67
3:F:1030:DT:C2'	3:F:1031:DT:H5"	2.24	0.67
1:A:196:ASP:HB3	1:A:202:SER:HA	1.75	0.67
1:A:214:LEU:HD23	1:A:220:PHE:CD2	2.30	0.67
4:A:2015:HOH:O	3:E:27:DT:H71	1.96	0.66
1:C:1216:LEU:HD23	1:C:1217:HIS:HE1	1.60	0.66
1:C:1237:ASN:CG	1:C:1238:PRO:HD3	2.16	0.66
2:B:10:DC:O2	3:E:28:DG:N2	2.23	0.66
3:E:35:DT:C2'	3:E:36:DA:C8	2.79	0.65
1:C:1161:SER:OG	1:C:1162:TYR:N	2.28	0.65
1:A:196:ASP:OD2	1:A:203:SER:HB2	1.95	0.65
1:A:222:ARG:NH1	4:A:2020:HOH:O	2.30	0.65
1:A:225:ASN:HB2	1:A:231:SER:OG	1.97	0.65
1:A:213:ASN:ND2	1:A:213:ASN:H	1.93	0.64
1:A:235:ILE:HD13	1:A:235:ILE:H	1.63	0.64
1:A:246:ALA:O	1:A:248:ARG:CD	2.45	0.64
3:E:35:DT:C4'	3:E:35:DT:OP1	2.45	0.64
2:B:10:DC:H2"	2:B:11:DA:C8	2.33	0.64
1:A:246:ALA:O	1:A:248:ARG:N	2.31	0.64
3:F:1030:DT:H2"	3:F:1031:DT:C5'	2.27	0.64
1:C:1221:MET:CE	1:C:1237:ASN:HD22	2.11	0.63
1:C:1161:SER:O	1:C:1165:LEU:HG	1.98	0.63
1:C:1177:ARG:O	1:C:1178:LEU:HD23	1.99	0.63
3:E:31:DT:H2"	3:E:32:DA:O5'	1.99	0.63
1:C:1216:LEU:HD23	1:C:1217:HIS:CE1	2.34	0.62
1:C:1237:ASN:HD22	1:C:1238:PRO:HD3	1.62	0.62
1:C:1180:LEU:O	1:C:1183:ILE:HB	1.98	0.62
1:C:1212:HIS:NE2	3:F:1031:DT:O4	2.33	0.62
1:A:160:LEU:CD1	1:A:165:LEU:CD2	2.75	0.61
1:A:176:LYS:NZ	1:A:236:ILE:H	1.98	0.61
3:F:1025:DG:H2"	3:F:1026:DT:O5'	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:HIS:N	1:A:217:HIS:CD2	2.66	0.61
2:D:1011:DA:H2''	2:D:1012:DA:C5'	2.30	0.61
1:A:184:TYR:O	1:A:188:VAL:HG23	2.00	0.61
2:B:10:DC:H2''	2:B:11:DA:N7	2.15	0.61
3:F:1033:DC:H1'	3:F:1034:DA:N7	2.15	0.60
1:A:176:LYS:HD2	1:C:1175:ASP:OD1	2.02	0.60
1:C:1191:VAL:HG13	1:C:1192:PRO:HD2	1.84	0.60
1:C:1235:ILE:H	1:C:1235:ILE:HD13	1.65	0.60
1:A:196:ASP:OD1	1:A:203:SER:CB	2.48	0.60
1:C:1210:ILE:O	1:C:1214:LEU:HG	2.01	0.60
3:E:28:DG:C1'	3:E:29:DT:H5''	2.33	0.59
1:C:1159:ASN:HD22	1:C:1159:ASN:N	2.01	0.59
3:F:1035:DT:C2	3:F:1036:DA:C8	2.91	0.59
3:F:1032:DA:H2'	3:F:1033:DC:H2'	1.85	0.58
3:F:1033:DC:H4'	3:F:1034:DA:C5'	2.33	0.58
2:D:1011:DA:H2''	2:D:1012:DA:H5''	1.85	0.58
1:C:1185:GLU:O	1:C:1189:ARG:HD3	2.04	0.58
2:B:6:DT:H2''	2:B:7:DA:C8	2.39	0.58
3:F:1027:DT:H2''	3:F:1028:DG:H5''	1.85	0.57
1:A:179:THR:O	1:A:180:LEU:C	2.42	0.57
2:D:1004:DT:H2''	2:D:1005:DG:C8	2.39	0.57
1:C:1216:LEU:HG	1:C:1217:HIS:ND1	2.18	0.57
2:B:9:DA:C2'	2:B:10:DC:O5'	2.53	0.56
1:A:212:HIS:CD2	3:E:30:DT:O4	2.57	0.56
1:C:1199:ASP:HA	1:C:1202:SER:HB3	1.88	0.56
3:F:1032:DA:C2'	3:F:1033:DC:O5'	2.52	0.56
2:D:1011:DA:H61	3:F:1027:DT:H3	1.53	0.56
1:A:221:MET:O	1:A:235:ILE:HD13	2.07	0.55
1:C:1178:LEU:O	1:C:1234:TRP:N	2.39	0.55
1:C:1188:VAL:HB	1:C:1196:ASP:OD2	2.06	0.55
3:F:1030:DT:H2''	3:F:1031:DT:H5''	1.85	0.55
1:A:188:VAL:CG1	1:A:198:GLY:N	2.63	0.55
1:A:177:ARG:HH22	1:C:1237:ASN:HB2	1.71	0.55
1:A:252:VAL:HG12	1:A:253:SER:H	1.72	0.55
1:C:1222:ARG:HH21	1:C:1222:ARG:HB2	1.72	0.55
1:C:1177:ARG:NH2	1:C:1177:ARG:HG2	2.22	0.54
1:C:1221:MET:HE3	1:C:1237:ASN:HD22	1.70	0.54
2:B:11:DA:C2'	2:B:12:DA:H5''	2.36	0.54
1:C:1162:TYR:O	1:C:1166:ILE:HG12	2.07	0.54
1:C:1227:GLY:C	1:C:1229:GLY:N	2.61	0.54
1:A:217:HIS:CD2	1:A:217:HIS:H	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:THR:H	1:A:182:GLN:HB2	1.72	0.54
2:D:1004:DT:H2''	2:D:1005:DG:H8	1.72	0.54
1:A:162:TYR:CE2	1:A:194:PHE:HZ	2.25	0.53
1:C:1192:PRO:HG2	1:C:1193:TYR:H	1.74	0.53
2:D:1005:DG:O5'	2:D:1005:DG:H8	1.92	0.53
1:A:223:VAL:HB	1:C:1223:VAL:HB	1.91	0.53
2:B:11:DA:H2''	2:B:12:DA:H5'	1.91	0.53
1:C:1194:PHE:N	1:C:1194:PHE:CD2	2.76	0.53
2:B:3:DA:H2''	2:B:4:DT:H5'	1.91	0.52
1:A:188:VAL:HG21	1:A:197:LYS:HB3	1.91	0.52
2:D:1002:DT:O4	3:F:1036:DA:N1	2.43	0.52
1:C:1166:ILE:O	1:C:1169:ALA:HB3	2.10	0.51
2:D:1002:DT:C4	3:F:1036:DA:N1	2.78	0.51
1:C:1218:SER:O	1:C:1219:ARG:C	2.49	0.51
1:C:1159:ASN:H	1:C:1159:ASN:ND2	2.08	0.51
1:C:1164:ASP:O	1:C:1168:ARG:HG2	2.10	0.51
1:C:1207:LYS:HZ3	1:C:1207:LYS:HB3	1.76	0.51
3:F:1029:DT:C2'	3:F:1030:DT:H5'	2.32	0.51
1:C:1159:ASN:ND2	1:C:1159:ASN:N	2.59	0.51
1:C:1221:MET:CG	1:C:1235:ILE:HD11	2.41	0.50
1:C:1184:TYR:CE1	1:C:1207:LYS:HB2	2.46	0.50
2:D:1011:DA:H2''	2:D:1012:DA:O5'	2.11	0.50
2:D:1005:DG:C2'	2:D:1006:DT:O5'	2.58	0.50
3:E:28:DG:H2''	3:E:29:DT:C5'	2.42	0.50
3:F:1031:DT:H5'	3:F:1031:DT:H6	1.76	0.50
1:C:1184:TYR:OH	1:C:1211:ARG:HG3	2.12	0.49
1:A:252:VAL:CG1	1:A:253:SER:H	2.25	0.49
1:A:213:ASN:N	1:A:213:ASN:ND2	2.55	0.49
2:D:1009:DA:H1'	2:D:1010:DC:OP1	2.12	0.49
3:E:28:DG:C2'	3:E:29:DT:H5''	2.42	0.49
1:C:1198:GLY:O	1:C:1199:ASP:CB	2.60	0.49
1:A:197:LYS:O	1:A:198:GLY:O	2.31	0.48
1:C:1227:GLY:O	1:C:1229:GLY:N	2.46	0.48
1:A:177:ARG:NH2	1:C:1237:ASN:HB2	2.27	0.48
1:A:207:LYS:HG2	1:A:211:ARG:HH11	1.76	0.48
1:C:1162:TYR:HA	1:C:1165:LEU:HD12	1.95	0.48
1:A:176:LYS:HE2	1:A:236:ILE:N	2.24	0.48
1:C:1179:THR:HG22	1:C:1232:SER:O	2.13	0.48
1:C:1166:ILE:HB	1:C:1220:PHE:CE2	2.48	0.48
3:E:25:DG:C8	3:E:26:DT:H72	2.48	0.48
3:E:34:DA:H2''	3:E:35:DT:O5'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1167:THR:OG1	1:C:1219:ARG:HD3	2.13	0.48
1:A:180:LEU:HB3	1:A:184:TYR:HE2	1.78	0.47
1:C:1218:SER:O	1:C:1220:PHE:N	2.48	0.47
1:A:180:LEU:HD22	3:E:27:DT:H3'	1.97	0.47
1:A:219:ARG:O	1:A:236:ILE:HD13	2.15	0.47
1:C:1221:MET:CE	1:C:1237:ASN:ND2	2.75	0.47
1:C:1221:MET:HG2	1:C:1222:ARG:H	1.75	0.47
1:C:1217:HIS:N	1:C:1217:HIS:ND1	2.63	0.47
1:C:1184:TYR:CZ	1:C:1207:LYS:HB2	2.50	0.47
2:B:13:DC:O2	3:E:25:DG:N1	2.47	0.47
1:C:1221:MET:HE1	1:C:1237:ASN:ND2	2.31	0.46
1:C:1212:HIS:HA	3:F:1029:DT:H72	1.97	0.46
1:A:179:THR:OG1	1:A:182:GLN:NE2	2.48	0.46
1:A:225:ASN:CB	1:A:231:SER:OG	2.64	0.46
3:F:1035:DT:H2''	3:F:1036:DA:H8	1.80	0.46
1:C:1218:SER:C	1:C:1220:PHE:N	2.67	0.46
1:C:1178:LEU:O	1:C:1233:TRP:HA	2.16	0.46
1:A:196:ASP:OD2	1:A:206:TRP:CE2	2.68	0.45
1:C:1221:MET:CG	1:C:1222:ARG:N	2.76	0.45
1:C:1161:SER:OG	2:D:1004:DT:O3'	2.35	0.45
1:C:1187:MET:HA	1:C:1191:VAL:HG23	1.98	0.45
1:C:1165:LEU:O	1:C:1166:ILE:C	2.53	0.45
1:C:1206:TRP:O	1:C:1209:SER:CB	2.65	0.45
2:B:4:DT:N3	3:E:34:DA:C2	2.75	0.45
1:C:1191:VAL:CG1	1:C:1192:PRO:HD2	2.45	0.45
1:A:212:HIS:HD2	3:E:30:DT:C4	2.35	0.45
2:B:13:DC:N3	3:E:25:DG:O6	2.50	0.44
1:A:169:ALA:HB2	1:A:186:TRP:CE3	2.52	0.44
1:A:194:PHE:HE2	1:A:206:TRP:CB	2.30	0.44
1:A:224:GLN:HB2	1:C:1226:GLU:OE1	2.18	0.44
1:C:1187:MET:O	1:C:1191:VAL:HG23	2.17	0.44
3:E:31:DT:H6	3:E:31:DT:H5'	1.83	0.44
1:A:176:LYS:HD2	1:C:1175:ASP:CB	2.48	0.44
1:A:250:ARG:HE	1:A:252:VAL:HG13	1.83	0.44
2:B:13:DC:N3	3:E:25:DG:C6	2.86	0.44
2:D:1008:DA:H2''	2:D:1009:DA:O5'	2.17	0.44
1:C:1157:MET:CB	2:D:1005:DG:H3'	2.49	0.43
1:A:217:HIS:N	1:A:217:HIS:HD2	2.16	0.43
1:A:222:ARG:HD3	1:A:232:SER:OG	2.19	0.43
1:A:251:ALA:C	1:A:252:VAL:CG2	2.83	0.43
1:C:1227:GLY:O	1:C:1228:THR:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LEU:HA	1:A:220:PHE:CD1	2.53	0.43
2:B:11:DA:H1'	2:B:12:DA:H5''	2.01	0.43
2:D:1009:DA:H2'	2:D:1010:DC:C5	2.52	0.43
1:C:1196:ASP:C	1:C:1197:LYS:HG3	2.39	0.43
2:D:1002:DT:C2'	2:D:1003:DA:C8	2.99	0.43
1:A:247:PRO:O	1:A:249:ARG:N	2.52	0.43
1:C:1187:MET:CA	1:C:1191:VAL:HG23	2.49	0.43
1:A:167:THR:O	1:A:170:ILE:HG22	2.19	0.42
1:C:1161:SER:C	1:C:1165:LEU:HG	2.40	0.42
1:A:224:GLN:HB2	1:C:1226:GLU:CD	2.39	0.42
3:F:1033:DC:H4'	3:F:1034:DA:H5'	2.01	0.42
1:A:196:ASP:HB2	1:A:206:TRP:CZ2	2.54	0.42
2:D:1004:DT:H1'	2:D:1005:DG:H5'	2.01	0.42
1:A:188:VAL:HG11	1:A:197:LYS:N	2.34	0.42
3:E:36:DA:C6	3:E:37:DG:C6	3.07	0.42
3:F:1033:DC:P	3:F:1033:DC:H3'	2.58	0.42
1:A:179:THR:O	1:A:183:ILE:HG13	2.20	0.42
1:A:196:ASP:O	1:A:202:SER:N	2.51	0.42
1:A:167:THR:C	1:A:170:ILE:HG22	2.39	0.42
1:C:1184:TYR:O	1:C:1187:MET:HB2	2.20	0.42
2:B:4:DT:C4	3:E:34:DA:N1	2.88	0.42
1:A:180:LEU:O	1:A:181:SER:C	2.59	0.42
1:A:194:PHE:HE2	1:A:206:TRP:CG	2.38	0.42
1:A:251:ALA:HB3	1:A:252:VAL:H	1.54	0.42
2:D:1010:DC:H4'	2:D:1011:DA:OP1	2.20	0.42
3:E:25:DG:N2	3:E:26:DT:C2	2.88	0.42
1:C:1207:LYS:O	1:C:1208:ASN:C	2.59	0.41
1:C:1201:ASN:C	1:C:1201:ASN:ND2	2.72	0.41
2:B:13:DC:C2	3:E:25:DG:N1	2.81	0.41
1:C:1187:MET:HB3	1:C:1191:VAL:HG21	2.03	0.41
1:A:238:PRO:HD3	4:A:2031:HOH:O	2.20	0.41
1:C:1207:LYS:CB	1:C:1207:LYS:NZ	2.78	0.41
1:C:1207:LYS:O	1:C:1210:ILE:N	2.52	0.41
1:C:1221:MET:HB3	1:C:1235:ILE:HD11	2.02	0.41
1:A:191:VAL:O	1:A:192:PRO:C	2.58	0.41
2:B:4:DT:H2''	2:B:5:DG:O5'	2.21	0.41
1:C:1161:SER:O	1:C:1165:LEU:N	2.53	0.41
1:C:1173:SER:HA	1:C:1174:PRO:HD3	1.96	0.41
1:C:1206:TRP:O	1:C:1209:SER:N	2.53	0.41
1:A:204:ALA:HB1	1:A:205:GLY:H	1.55	0.40
1:C:1210:ILE:HG13	1:C:1211:ARG:N	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:VAL:O	1:A:193:TYR:N	2.54	0.40
1:A:196:ASP:HB2	1:A:206:TRP:HZ2	1.85	0.40
1:C:1239:ASP:HA	4:C:2064:HOH:O	2.20	0.40
1:A:224:GLN:HB2	1:C:1226:GLU:OE2	2.21	0.40
1:C:1244:GLY:C	1:C:1246:ALA:N	2.74	0.40
1:A:212:HIS:CE1	2:B:6:DT:O4	2.74	0.40
1:C:1171:GLU:C	1:C:1173:SER:N	2.75	0.40
1:C:1225:ASN:HB2	1:C:1231:SER:OG	2.21	0.40
3:F:1032:DA:H2''	3:F:1033:DC:C2'	2.48	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	95/97 (98%)	64 (67%)	17 (18%)	14 (15%)	0	0
1	C	90/97 (93%)	65 (72%)	13 (14%)	12 (13%)	0	0
All	All	185/194 (95%)	129 (70%)	30 (16%)	26 (14%)	0	0

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	GLY
1	A	204	ALA
1	A	217	HIS
1	A	238	PRO
1	A	247	PRO
1	A	249	ARG
1	A	252	VAL
1	C	1160	LEU
1	C	1197	LYS

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Mol	Chain	Res	Type
1	C	1200	SER
1	C	1238	PRO
1	C	1242	LYS
1	C	1243	SER
1	C	1246	ALA
1	C	1247	PRO
1	A	191	VAL
1	A	205	GLY
1	A	250	ARG
1	C	1203	SER
1	C	1228	THR
1	A	192	PRO
1	A	158	GLY
1	A	227	GLY
1	A	244	GLY
1	C	1205	GLY
1	C	1192	PRO

5.3.2 Protein sidechains ⓘ

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	84/84 (100%)	64 (76%)	20 (24%)	0	2
1	C	74/84 (88%)	51 (69%)	23 (31%)	0	0
All	All	158/168 (94%)	115 (73%)	43 (27%)	0	1

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	MET
1	A	160	LEU
1	A	161	SER
1	A	162	TYR
1	A	164	ASP
1	A	165	LEU

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Mol	Chain	Res	Type
1	A	177	ARG
1	A	195	LYS
1	A	197	LYS
1	A	203	SER
1	A	208	ASN
1	A	213	ASN
1	A	217	HIS
1	A	219	ARG
1	A	220	PHE
1	A	230	LYS
1	A	235	ILE
1	A	238	PRO
1	A	250	ARG
1	A	252	VAL
1	C	1159	ASN
1	C	1160	LEU
1	C	1164	ASP
1	C	1176	LYS
1	C	1177	ARG
1	C	1180	LEU
1	C	1182	GLN
1	C	1193	TYR
1	C	1194	PHE
1	C	1195	LYS
1	C	1196	ASP
1	C	1197	LYS
1	C	1202	SER
1	C	1207	LYS
1	C	1209	SER
1	C	1213	ASN
1	C	1215	SER
1	C	1217	HIS
1	C	1222	ARG
1	C	1226	GLU
1	C	1233	TRP
1	C	1235	ILE
1	C	1238	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN

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Mol	Chain	Res	Type
1	A	208	ASN
1	A	212	HIS
1	A	213	ASN
1	A	217	HIS
1	C	1159	ASN
1	C	1182	GLN
1	C	1201	ASN
1	C	1208	ASN
1	C	1224	GLN
1	C	1237	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	247:PRO	C	248:ARG	N	1.16

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	97/97 (100%)	0.40	9 (9%) 8 6	0, 19, 61, 70	0
1	C	92/97 (94%)	0.30	3 (3%) 46 46	1, 18, 48, 58	0
2	B	13/13 (100%)	-0.60	0 100 100	3, 8, 18, 20	0
2	D	13/13 (100%)	-0.41	0 100 100	9, 14, 24, 27	0
3	E	13/13 (100%)	-0.58	0 100 100	3, 8, 23, 23	0
3	F	13/13 (100%)	-0.32	0 100 100	4, 17, 26, 26	0
All	All	241/246 (97%)	0.17	12 (4%) 28 27	0, 17, 56, 70	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1200	SER	4.9
1	C	1199	ASP	4.7
1	A	228	THR	4.1
1	A	247	PRO	3.7
1	A	246	ALA	3.1
1	A	251	ALA	2.6
1	C	1202	SER	2.4
1	A	238	PRO	2.2
1	A	253	SER	2.2
1	A	252	VAL	2.1
1	A	201	ASN	2.1
1	A	249	ARG	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 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.