Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:55 AM GMT

PDB ID	:	2ESN
Title	:	The crystal structure of probable transcriptional regulator PA0477 from Pseudomonas aeruginosa
Authors	:	Lunin, V.V.; Chang, C.; Skarina, T.; Gorodischenskaya, E.; Edwards, A.M.; Joachimiak, A.; Savchenko, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2005-10-26
Resolution	:	2.10 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:

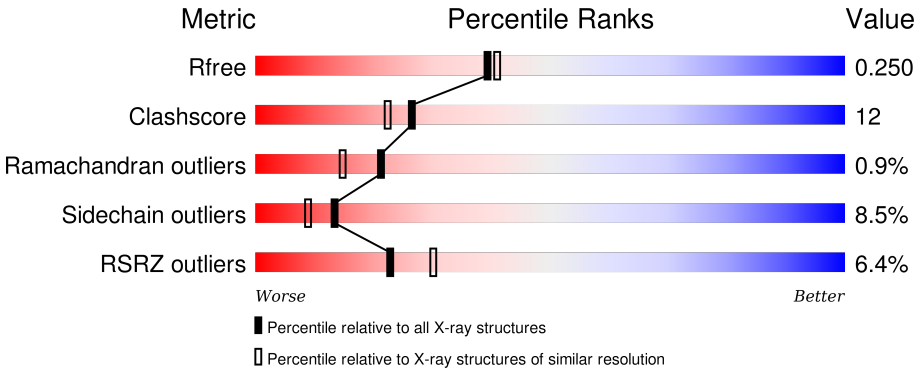
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	310	5% 74% 19%
1	B	310	5% 72% 18% 5%
1	C	310	4% 73% 19%
1	D	310	11% 72% 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10202 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 probable transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	2	0
			2360	1498	445	414	3			
1	C	298	Total	C	N	O	S	0	3	0
			2363	1502	449	409	3			
1	B	300	Total	C	N	O	S	0	0	0
			2347	1493	437	414	3			
1	D	298	Total	C	N	O	S	0	3	0
			2362	1500	444	415	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	GB 9946339
A	0	HIS	-	CLONING ARTIFACT	GB 9946339
B	-1	GLY	-	CLONING ARTIFACT	GB 9946339
B	0	HIS	-	CLONING ARTIFACT	GB 9946339
C	-1	GLY	-	CLONING ARTIFACT	GB 9946339
C	0	HIS	-	CLONING ARTIFACT	GB 9946339
D	-1	GLY	-	CLONING ARTIFACT	GB 9946339
D	0	HIS	-	CLONING ARTIFACT	GB 9946339

- Molecule 2 is water.

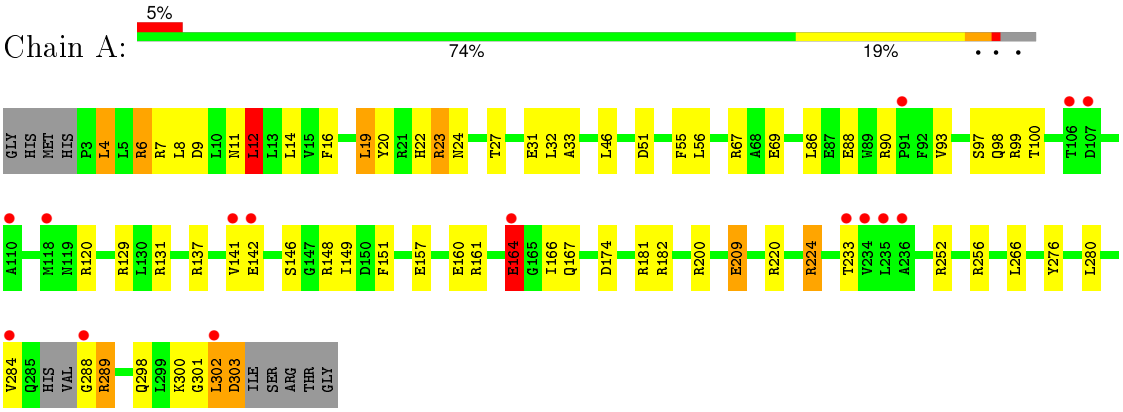
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	224	Total	O	0	0
			224	224		
2	B	201	Total	O	0	0
			201	201		
2	C	204	Total	O	0	0
			204	204		
2	D	141	Total	O	0	0
			141	141		

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 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.

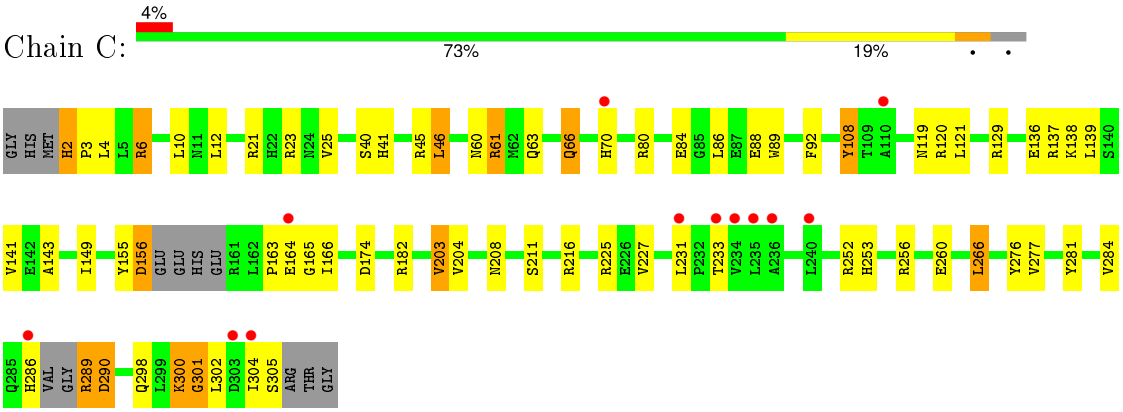
- Molecule 1: probable transcriptional regulator

Chain A:



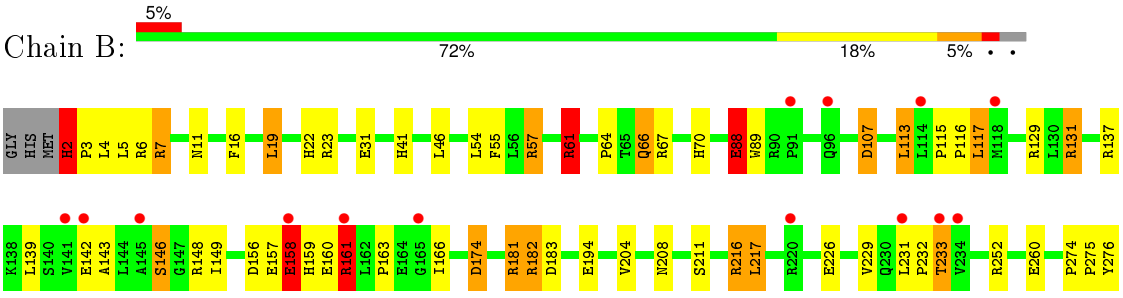
- Molecule 1: probable transcriptional regulator

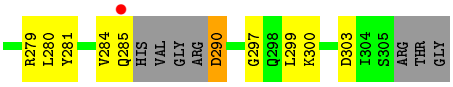
Chain C:



- Molecule 1: probable transcriptional regulator

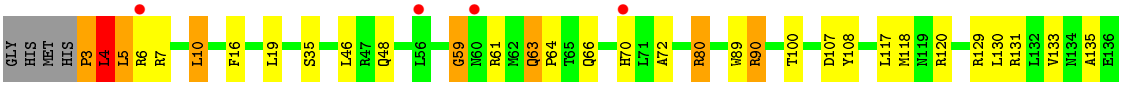
Chain B:

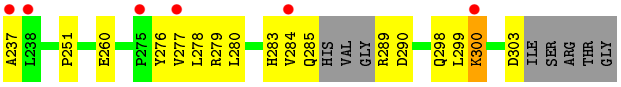




• Molecule 1: probable transcriptional regulator

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	97.03Å 171.21Å 86.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 34.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.1 (50.00-2.10) 97.1 (34.01-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.194 , 0.251 0.193 , 0.250	Depositor DCC
R_{free} test set	2466 reflections (3.09%)	DCC
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 65.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 82383 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10202	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.19% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.02	0/2414	1.01	8/3280 (0.2%)
1	B	1.01	1/2402 (0.0%)	1.03	16/3268 (0.5%)
1	C	1.07	2/2418 (0.1%)	0.98	6/3286 (0.2%)
1	D	0.92	0/2417	0.92	3/3286 (0.1%)
All	All	1.01	3/9651 (0.0%)	0.98	33/13120 (0.3%)

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	B	0	3
1	C	0	1
1	D	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	108	TYR	CD2-CE2	6.75	1.49	1.39
1	C	80	ARG	CG-CD	5.16	1.64	1.51
1	B	194	GLU	CG-CD	5.10	1.59	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	ARG	NE-CZ-NH1	-8.89	115.86	120.30
1	A	224	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	A	181	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	D	162	LEU	CA-CB-CG	7.22	131.90	115.30
1	C	46	LEU	CA-CB-CG	7.22	131.90	115.30
1	B	181	ARG	NE-CZ-NH2	7.19	123.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	117	LEU	CB-CG-CD2	7.12	123.11	111.00
1	B	131	ARG	NE-CZ-NH2	-6.59	117.01	120.30
1	B	182	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	216	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	181	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	B	131	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	266	LEU	CA-CB-CG	6.21	129.58	115.30
1	B	174	ASP	CB-CG-OD1	6.13	123.82	118.30
1	D	4	LEU	CA-CB-CG	6.03	129.16	115.30
1	B	113	LEU	CB-CG-CD2	6.00	121.19	111.00
1	B	61	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	B	233	THR	CB-CA-C	-5.89	95.71	111.60
1	C	121	LEU	CB-CG-CD1	5.79	120.84	111.00
1	B	161	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	129	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	C	21	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	252	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	12	LEU	CB-CG-CD1	5.53	120.39	111.00
1	C	225	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	C	266	LEU	CA-CB-CG	5.38	127.67	115.30
1	A	209	GLU	CA-CB-CG	5.37	125.21	113.40
1	D	80	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	182	ARG	NE-CZ-NH1	-5.31	117.65	120.30
1	B	216	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	45	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	A	200	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	B	159	HIS	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	158	GLU	Peptide
1	B	2	HIS	Peptide
1	B	284	VAL	Peptide
1	C	60	ASN	Peptide
1	D	3	PRO	Peptide
1	D	59	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	2360	0	2364	50	1
1	B	2347	0	2346	66	1
1	C	2363	0	2370	67	1
1	D	2362	0	2361	67	0
2	A	224	0	0	13	0
2	B	201	0	0	17	0
2	C	204	0	0	12	0
2	D	141	0	0	13	0
All	All	10202	0	9441	231	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 12.

All (231) 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:D:3:PRO:N	1:D:4:LEU:HB2	1.63	1.12
1:C:23:ARG:HH21	1:C:61:ARG:HH22	1.04	1.01
1:D:117:LEU:HG	1:D:118:MET:HE2	1.51	0.93
1:B:174:ASP:HB3	1:B:276:TYR:CZ	2.08	0.89
1:B:285:GLN:HA	2:B:407:HOH:O	1.75	0.86
1:C:120[A]:ARG:NH2	1:C:298:GLN:O	2.08	0.85
1:D:70:HIS:NE2	2:D:440:HOH:O	2.10	0.83
1:C:25:VAL:HB	2:C:507:HOH:O	1.78	0.83
1:B:158:GLU:O	1:B:158:GLU:HG3	1.76	0.83
1:C:182:ARG:HH22	1:C:260:GLU:CD	1.81	0.82
1:D:138:LYS:H	1:D:138:LYS:HD2	1.43	0.82
1:C:182:ARG:NH2	1:C:260:GLU:OE2	2.13	0.81
1:B:107:ASP:HB2	1:D:233[B]:THR:HG21	1.64	0.80
1:A:67:ARG:HH12	1:D:90:ARG:HG3	1.46	0.79
1:C:86:LEU:HD12	1:B:5:LEU:HD23	1.64	0.79
1:C:141:VAL:HG22	1:C:166:ILE:HD11	1.63	0.79
1:A:51:ASP:OD2	1:D:90:ARG:NH2	2.17	0.78
1:C:300:LYS:C	1:C:302:LEU:H	1.87	0.77
1:B:67:ARG:HG2	2:B:395:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ARG:NH2	1:C:61:ARG:HH22	1.82	0.77
1:B:2:HIS:N	1:B:3:PRO:HA	2.00	0.77
1:D:138:LYS:HD2	1:D:138:LYS:N	1.97	0.76
1:B:66:GLN:CD	1:B:66:GLN:H	1.86	0.76
1:D:138:LYS:H	1:D:138:LYS:CD	1.99	0.76
1:A:9:ASP:HB3	1:A:12:LEU:HD22	1.67	0.75
1:A:302:LEU:HB3	2:A:521:HOH:O	1.85	0.75
1:B:290:ASP:N	2:B:504:HOH:O	2.20	0.75
1:C:300:LYS:O	1:C:302:LEU:N	2.21	0.74
1:C:10:LEU:H	1:B:11:ASN:HD21	1.35	0.74
1:C:86:LEU:CD1	1:B:5:LEU:HD23	2.18	0.74
1:C:41:HIS:HB2	2:C:431:HOH:O	1.86	0.73
1:A:20:TYR:O	1:A:23:ARG:HD3	1.88	0.73
1:C:66:GLN:OE1	1:C:70[B]:HIS:CE1	2.42	0.72
1:D:233[B]:THR:CG2	2:D:447:HOH:O	2.38	0.72
1:C:165:GLY:HA2	1:C:284:VAL:HG22	1.72	0.72
1:B:157:GLU:O	1:B:160:GLU:HG3	1.89	0.72
1:C:66:GLN:OE1	1:C:70[B]:HIS:HE1	1.72	0.71
1:A:141:VAL:HG13	1:A:166:ILE:HD11	1.71	0.71
1:D:117:LEU:HD23	1:D:118:MET:HE3	1.72	0.71
1:D:70:HIS:CE1	2:D:440:HOH:O	2.44	0.70
1:C:174:ASP:HB3	1:C:276:TYR:CZ	2.26	0.70
1:C:141:VAL:HG22	1:C:166:ILE:CD1	2.21	0.70
1:D:170:ASP:OD1	1:D:279:ARG:HD3	1.92	0.70
1:A:256:ARG:NH1	2:A:520:HOH:O	2.25	0.69
1:D:117:LEU:HD23	1:D:118:MET:CE	2.22	0.69
2:A:443:HOH:O	1:D:66:GLN:HB3	1.91	0.69
1:A:24:ASN:OD1	1:A:27:THR:HG22	1.93	0.69
1:A:67:ARG:NH1	1:D:90:ARG:HG3	2.07	0.69
1:C:86:LEU:HD12	1:B:5:LEU:CD2	2.24	0.68
1:B:66:GLN:HG2	2:B:395:HOH:O	1.95	0.66
1:D:233[B]:THR:HG21	2:D:447:HOH:O	1.96	0.66
1:A:174:ASP:HB3	1:A:276:TYR:CZ	2.30	0.66
1:C:119:ASN:ND2	1:C:120[B]:ARG:HH21	1.95	0.65
1:D:120:ARG:HD3	1:D:298:GLN:HE22	1.60	0.65
1:B:260:GLU:HG2	2:B:505:HOH:O	1.96	0.64
1:D:80:ARG:HD3	2:D:444:HOH:O	1.98	0.64
1:D:117:LEU:CD2	1:D:118:MET:CE	2.75	0.64
1:A:4:LEU:HB2	2:A:428:HOH:O	1.98	0.63
1:B:139:LEU:HD21	1:B:166:ILE:HG13	1.78	0.63
1:B:161:ARG:HG2	1:B:161:ARG:HH11	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:HIS:HA	1:C:289:ARG:HD3	1.80	0.62
1:A:11:ASN:HD21	1:D:10:LEU:H	1.47	0.62
1:D:59:GLY:HA3	1:D:61:ARG:H	1.65	0.61
1:D:155:TYR:HB3	1:D:277:VAL:O	2.00	0.61
1:B:57:ARG:NH1	1:B:57:ARG:HG2	2.16	0.61
1:C:23:ARG:HH21	1:C:61:ARG:NH2	1.87	0.61
1:C:3:PRO:HB2	2:C:482:HOH:O	2.00	0.61
1:A:302:LEU:CD2	1:A:303:ASP:H	2.15	0.60
1:D:35:SER:HB2	2:D:389:HOH:O	2.01	0.60
1:B:161:ARG:CG	1:B:161:ARG:HH11	2.14	0.60
1:D:108:TYR:HB2	1:D:234:VAL:HG21	1.84	0.60
1:C:300:LYS:C	1:C:302:LEU:N	2.55	0.59
1:D:3:PRO:N	1:D:4:LEU:CB	2.53	0.59
1:D:284:VAL:O	1:D:285:GLN:HB2	2.01	0.59
1:B:70:HIS:HB2	2:B:414:HOH:O	2.03	0.58
1:C:2:HIS:CD2	1:C:3:PRO:HD2	2.39	0.57
1:D:190:ALA:HB1	2:D:443:HOH:O	2.03	0.57
1:A:148:ARG:HD2	2:A:500:HOH:O	2.02	0.57
1:C:252:ARG:NH2	1:C:256:ARG:HD2	2.19	0.57
1:B:57:ARG:HH11	1:B:57:ARG:CG	2.17	0.57
1:B:2:HIS:N	1:B:3:PRO:CA	2.68	0.57
1:D:117:LEU:CG	1:D:118:MET:HE2	2.31	0.57
1:C:12:LEU:HB3	1:C:46:LEU:HD13	1.87	0.57
1:B:88:GLU:HB3	1:B:89:TRP:CE3	2.40	0.57
1:D:16:PHE:HB2	1:D:46:LEU:HD21	1.87	0.57
1:A:19:LEU:HD13	1:A:55:PHE:CD1	2.40	0.57
1:D:117:LEU:HG	1:D:118:MET:CE	2.31	0.56
1:A:22:HIS:NE2	1:A:31:GLU:OE2	2.24	0.56
1:D:174:ASP:HB3	1:D:276:TYR:CZ	2.41	0.56
1:C:84:GLU:HG2	2:C:492:HOH:O	2.05	0.56
1:A:157:GLU:O	1:A:160:GLU:HG3	2.06	0.56
1:D:120:ARG:HD3	1:D:298:GLN:NE2	2.20	0.56
1:D:155:TYR:CB	1:D:277:VAL:O	2.54	0.56
1:A:93:VAL:HG21	2:A:529:HOH:O	2.06	0.55
1:A:164:GLU:OE2	1:A:164:GLU:HA	2.07	0.55
1:C:10:LEU:H	1:B:11:ASN:ND2	2.01	0.55
1:B:57:ARG:HH11	1:B:57:ARG:HG2	1.72	0.55
1:C:108:TYR:HH	1:C:276:TYR:HH	1.55	0.55
1:A:146:SER:HB2	1:A:148:ARG:H	1.72	0.55
1:B:19:LEU:HD13	1:B:55:PHE:CD1	2.42	0.54
1:A:302:LEU:HD23	1:A:303:ASP:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:LEU:O	1:D:217:LEU:HD12	2.08	0.54
1:D:107:ASP:OD2	1:D:233[B]:THR:HG23	2.07	0.54
1:B:217:LEU:O	1:B:217:LEU:HD23	2.07	0.54
1:D:203:VAL:HG22	1:D:230:GLN:HG2	1.90	0.54
1:B:66:GLN:N	1:B:66:GLN:CD	2.60	0.53
1:B:66:GLN:NE2	2:B:452:HOH:O	2.42	0.53
1:C:163:PRO:HB2	1:C:166:ILE:HD13	1.90	0.53
1:D:203:VAL:HG13	1:D:227:VAL:HG13	1.90	0.53
1:D:168:ALA:HA	1:D:280:LEU:O	2.09	0.52
1:A:97:SER:OG	1:A:99:ARG:HG2	2.08	0.52
1:A:16:PHE:HB2	1:A:46:LEU:HD21	1.91	0.52
1:B:217:LEU:C	1:B:217:LEU:HD23	2.29	0.52
1:B:156:ASP:OD2	1:B:279:ARG:NH1	2.42	0.52
1:C:120[A]:ARG:HH12	1:C:301:GLY:HA3	1.75	0.51
1:B:107:ASP:HB2	2:D:447:HOH:O	2.10	0.51
1:C:165:GLY:HA2	1:C:284:VAL:CG2	2.38	0.51
1:B:208:ASN:HB3	2:D:442:HOH:O	2.09	0.51
1:A:100:THR:HA	1:A:129[B]:ARG:O	2.10	0.51
1:B:142:GLU:O	1:B:146:SER:OG	2.28	0.51
1:A:22:HIS:HB3	1:A:27:THR:HG23	1.93	0.50
1:C:155:TYR:HE1	2:C:392:HOH:O	1.93	0.50
1:D:145:ALA:HA	1:D:283:HIS:CD2	2.46	0.50
1:B:22:HIS:NE2	1:B:31:GLU:OE2	2.28	0.50
1:C:203:VAL:HG13	1:C:227:VAL:HG13	1.93	0.50
1:C:165:GLY:CA	1:C:284:VAL:HG22	2.40	0.50
1:B:61:ARG:HD2	2:B:503:HOH:O	2.10	0.50
1:A:67:ARG:HB3	1:D:89:TRP:CZ3	2.47	0.50
1:D:289:ARG:HA	2:D:410:HOH:O	2.11	0.50
1:B:174:ASP:HB3	1:B:276:TYR:CE1	2.45	0.49
1:A:120:ARG:HH22	1:A:301:GLY:HA3	1.77	0.49
1:B:226:GLU:HB3	2:B:350:HOH:O	2.12	0.49
1:A:14:LEU:HD12	2:A:421:HOH:O	2.12	0.49
1:A:303:ASP:OD2	1:A:303:ASP:C	2.51	0.48
1:A:141:VAL:HG13	1:A:166:ILE:CD1	2.42	0.48
1:D:300:LYS:HG3	2:D:366:HOH:O	2.13	0.48
1:B:16:PHE:HB2	1:B:46:LEU:CD2	2.43	0.48
1:A:6:ARG:HD2	2:A:380:HOH:O	2.12	0.48
1:C:156:ASP:HB3	2:C:460:HOH:O	2.14	0.48
1:A:220:ARG:NH2	2:A:460:HOH:O	2.45	0.48
1:C:252:ARG:O	1:C:256:ARG:HG3	2.13	0.48
1:B:161:ARG:NH1	1:B:161:ARG:HG2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ASP:HB3	1:C:276:TYR:OH	2.13	0.48
1:B:208:ASN:O	1:D:131:ARG:NH2	2.47	0.47
1:C:63:GLN:HG2	2:C:496:HOH:O	2.14	0.47
1:C:6:ARG:HG3	1:C:6:ARG:HH21	1.79	0.47
1:D:182:ARG:HH12	1:D:260:GLU:CD	2.18	0.47
1:D:16:PHE:HB2	1:D:46:LEU:CD2	2.44	0.47
1:D:251:PRO:HB3	1:D:276:TYR:OH	2.14	0.47
1:D:135:ALA:HB1	2:D:395:HOH:O	2.14	0.47
1:D:280:LEU:HD22	1:D:299:LEU:HD22	1.97	0.46
1:B:279:ARG:HG3	1:B:281:TYR:CZ	2.50	0.46
1:D:138:LYS:CE	1:D:138:LYS:H	2.28	0.46
1:C:163:PRO:HB2	1:C:166:ILE:CD1	2.44	0.46
1:C:304:ILE:HG23	2:C:319:HOH:O	2.14	0.46
1:B:16:PHE:HB2	1:B:46:LEU:HD21	1.98	0.46
1:A:131:ARG:NH2	1:C:208:ASN:O	2.48	0.46
1:B:285:GLN:HB2	2:B:487:HOH:O	2.15	0.46
1:C:302:LEU:HD12	1:C:302:LEU:HA	1.82	0.46
1:C:6:ARG:HG3	1:C:6:ARG:NH2	2.30	0.46
1:A:137:ARG:HD2	2:A:525:HOH:O	2.16	0.45
1:A:9:ASP:O	1:A:12:LEU:HB2	2.16	0.45
1:D:133:VAL:HG12	2:D:442:HOH:O	2.16	0.45
1:A:98:GLN:OE1	1:A:129[B]:ARG:NH1	2.49	0.45
1:C:290:ASP:HB2	2:C:382:HOH:O	2.17	0.45
1:B:285:GLN:CG	2:B:407:HOH:O	2.65	0.45
1:C:119:ASN:ND2	1:C:120[B]:ARG:NH2	2.62	0.45
1:A:88:GLU:OE1	1:D:70:HIS:ND1	2.50	0.45
1:C:89:TRP:O	1:B:67:ARG:NH1	2.50	0.45
1:A:12:LEU:HB3	1:A:46:LEU:HD13	1.99	0.45
1:A:146:SER:CB	1:A:148:ARG:H	2.30	0.44
1:C:211:SER:O	1:C:216:ARG:NH1	2.50	0.44
1:C:204:VAL:HA	1:C:231:LEU:O	2.17	0.44
1:A:164:GLU:CA	1:A:164:GLU:OE2	2.65	0.44
1:D:233[B]:THR:HG22	1:D:236:ALA:H	1.82	0.44
1:D:120:ARG:HH11	1:D:298:GLN:NE2	2.15	0.44
1:B:54:LEU:O	1:B:64:PRO:HA	2.18	0.44
1:B:280:LEU:HD22	1:B:299:LEU:HD22	1.99	0.44
1:B:57:ARG:HH11	1:B:57:ARG:HB3	1.82	0.44
1:A:252:ARG:NH1	1:A:256:ARG:HD3	2.33	0.44
1:A:86:LEU:HD12	1:D:5:LEU:HD13	2.00	0.44
1:C:61:ARG:HB3	1:C:61:ARG:HE	1.20	0.44
1:B:211:SER:O	1:B:216:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:HIS:HE1	1:C:305:SER:HB2	1.83	0.44
1:C:119:ASN:HD21	1:C:120[B]:ARG:HH21	1.62	0.43
1:C:155:TYR:HB2	1:C:277:VAL:O	2.18	0.43
1:B:303:ASP:OD2	2:B:498:HOH:O	2.21	0.43
1:B:137:ARG:HD3	2:B:368:HOH:O	2.19	0.43
1:A:288:GLY:HA3	2:A:434:HOH:O	2.16	0.43
1:D:284:VAL:O	1:D:285:GLN:CB	2.66	0.43
1:C:86:LEU:CD1	1:B:5:LEU:CD2	2.89	0.43
1:A:32:LEU:O	1:A:33:ALA:HB3	2.18	0.43
1:A:174:ASP:HB3	1:A:276:TYR:OH	2.17	0.43
1:C:300:LYS:HD3	1:C:300:LYS:N	2.34	0.43
1:B:115:PRO:HB2	1:B:116:PRO:HD3	1.99	0.43
1:B:229:VAL:HA	1:D:130:LEU:O	2.18	0.43
1:D:117:LEU:CG	1:D:118:MET:CE	2.93	0.42
1:C:2:HIS:HD2	1:C:4:LEU:H	1.67	0.42
1:B:182:ARG:NH2	2:B:370:HOH:O	2.52	0.42
1:B:7:ARG:NH1	2:B:439:HOH:O	2.32	0.42
1:A:151:PHE:CG	1:A:280:LEU:HD11	2.54	0.42
1:B:297:GLY:HA2	1:B:300:LYS:HD2	2.02	0.42
1:D:203:VAL:HG22	1:D:230:GLN:CG	2.50	0.42
1:C:143:ALA:HB1	1:C:149:ILE:HD12	2.02	0.42
1:A:131:ARG:NH2	2:A:418:HOH:O	2.53	0.41
1:D:231:LEU:HD21	1:D:237:ALA:HB2	2.01	0.41
1:C:70[A]:HIS:HE2	1:B:88:GLU:HB2	1.84	0.41
1:D:59:GLY:CA	1:D:61:ARG:H	2.33	0.41
1:C:40:SER:HB2	2:C:463:HOH:O	2.20	0.41
1:C:86:LEU:O	1:C:89:TRP:HB3	2.20	0.41
1:B:274:PRO:HA	1:B:275:PRO:HD3	1.93	0.41
1:A:4:LEU:HD12	2:A:428:HOH:O	2.20	0.41
1:A:120:ARG:HH11	1:A:298:GLN:NE2	2.19	0.41
1:D:278:LEU:HA	1:D:278:LEU:HD23	1.89	0.41
1:A:284:VAL:HG22	1:A:284:VAL:O	2.21	0.41
1:B:143:ALA:HB1	1:B:149:ILE:HD12	2.02	0.41
1:D:100:THR:HA	1:D:129[A]:ARG:O	2.20	0.41
1:B:163:PRO:HA	2:B:477:HOH:O	2.21	0.41
1:C:138:LYS:HE3	1:C:281:TYR:CZ	2.56	0.41
1:B:157:GLU:OE2	1:B:216:ARG:HD2	2.21	0.41
1:B:161:ARG:CB	1:B:161:ARG:HH11	2.34	0.41
1:D:63:GLN:HA	1:D:64:PRO:HD3	1.95	0.40
1:D:138:LYS:HB3	1:D:207:TRP:CH2	2.56	0.40
1:C:141:VAL:HG13	1:C:166:ILE:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:PHE:HE1	1:D:72:ALA:HA	1.86	0.40
1:B:137:ARG:HB2	2:B:447:HOH:O	2.21	0.40
1:C:129:ARG:NH1	2:C:409:HOH:O	2.54	0.40
1:D:138:LYS:HB3	1:D:207:TRP:CZ2	2.57	0.40
1:C:260:GLU:HG2	2:C:478:HOH:O	2.20	0.40
1:C:92:PHE:HB2	1:C:290:ASP:HB3	2.03	0.40
1:B:204:VAL:HA	1:B:231:LEU:O	2.21	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)
1:B:41:HIS:ND1	1:B:183:ASP:OD1[1_556]	2.12	0.08
1:A:161[A]:ARG:NH1	1:C:289:ARG:N[4_456]	2.13	0.07

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	297/310 (96%)	286 (96%)	8 (3%)	3 (1%)	19	13
1	B	296/310 (96%)	286 (97%)	8 (3%)	2 (1%)	26	21
1	C	295/310 (95%)	283 (96%)	10 (3%)	2 (1%)	26	21
1	D	297/310 (96%)	281 (95%)	12 (4%)	4 (1%)	15	9
All	All	1185/1240 (96%)	1136 (96%)	38 (3%)	11 (1%)	21	15

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	LYS
1	D	141	VAL

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Mol	Chain	Res	Type
1	D	159	HIS
1	A	164	GLU
1	C	301	GLY
1	B	88	GLU
1	A	289	ARG
1	B	158	GLU
1	D	162	LEU
1	D	300	LYS
1	C	88	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	234/241 (97%)	214 (92%)	20 (8%)	13 9
1	B	234/241 (97%)	212 (91%)	22 (9%)	11 7
1	C	235/241 (98%)	220 (94%)	15 (6%)	22 18
1	D	235/241 (98%)	212 (90%)	23 (10%)	10 6
All	All	938/964 (97%)	858 (92%)	80 (8%)	13 9

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	6	ARG
1	A	7	ARG
1	A	8	LEU
1	A	12	LEU
1	A	19	LEU
1	A	23	ARG
1	A	56	LEU
1	A	69	GLU
1	A	90	ARG
1	A	142	GLU
1	A	149	ILE

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Mol	Chain	Res	Type
1	A	164	GLU
1	A	167	GLN
1	A	209	GLU
1	A	224	ARG
1	A	233	THR
1	A	289	ARG
1	A	302	LEU
1	A	303	ASP
1	C	2	HIS
1	C	6	ARG
1	C	61	ARG
1	C	66	GLN
1	C	136	GLU
1	C	137	ARG
1	C	139	LEU
1	C	156	ASP
1	C	164	GLU
1	C	203	VAL
1	C	233	THR
1	C	266	LEU
1	C	289	ARG
1	C	290	ASP
1	C	300	LYS
1	B	2	HIS
1	B	4	LEU
1	B	6	ARG
1	B	7	ARG
1	B	19	LEU
1	B	23	ARG
1	B	57	ARG
1	B	61	ARG
1	B	66	GLN
1	B	88	GLU
1	B	107	ASP
1	B	113	LEU
1	B	117	LEU
1	B	131	ARG
1	B	146	SER
1	B	148	ARG
1	B	161	ARG
1	B	181	ARG
1	B	217	LEU

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Mol	Chain	Res	Type
1	B	232	PRO
1	B	233	THR
1	B	290	ASP
1	D	4	LEU
1	D	5	LEU
1	D	6	ARG
1	D	7	ARG
1	D	10	LEU
1	D	19	LEU
1	D	48	GLN
1	D	63	GLN
1	D	90	ARG
1	D	137	ARG
1	D	138	LYS
1	D	141	VAL
1	D	148	ARG
1	D	162	LEU
1	D	177	VAL
1	D	186	ARG
1	D	203	VAL
1	D	210	ASP
1	D	224	ARG
1	D	233[A]	THR
1	D	233[B]	THR
1	D	290	ASP
1	D	303	ASP

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

Mol	Chain	Res	Type
1	A	11	ASN
1	A	167	GLN
1	A	230	GLN
1	A	298	GLN
1	C	2	HIS
1	C	41	HIS
1	C	48	GLN
1	C	119	ASN
1	B	11	ASN
1	B	159	HIS
1	D	63	GLN
1	D	96	GLN

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Mol	Chain	Res	Type
1	D	159	HIS
1	D	167	GLN
1	D	298	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	299/310 (96%)	0.08	15 (5%) 32 41	22, 39, 64, 86	0
1	B	300/310 (96%)	0.25	15 (5%) 32 41	25, 41, 64, 79	0
1	C	298/310 (96%)	0.11	12 (4%) 42 51	21, 37, 63, 81	0
1	D	298/310 (96%)	0.51	34 (11%) 7 9	27, 50, 78, 96	0
All	All	1195/1240 (96%)	0.24	76 (6%) 23 30	21, 41, 70, 96	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	60	ASN	7.4
1	D	141	VAL	7.1
1	D	159	HIS	6.5
1	D	284	VAL	6.2
1	D	233[A]	THR	5.3
1	A	288	GLY	5.0
1	D	158	GLU	4.8
1	A	141	VAL	4.7
1	D	145	ALA	3.9
1	D	162	LEU	3.8
1	D	156	ASP	3.6
1	D	231	LEU	3.4
1	D	300	LYS	3.3
1	C	164	GLU	3.2
1	D	56	LEU	3.2
1	D	236	ALA	3.1
1	B	91	PRO	3.1
1	B	220	ARG	3.1
1	B	158	GLU	3.0
1	B	165	GLY	3.0
1	D	161	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	285	GLN	3.0
1	D	235	LEU	3.0
1	D	234	VAL	2.9
1	B	233	THR	2.9
1	D	275	PRO	2.9
1	A	164	GLU	2.9
1	C	233	THR	2.8
1	A	236	ALA	2.8
1	B	118	MET	2.8
1	A	91	PRO	2.7
1	D	221	SER	2.7
1	D	165	GLY	2.7
1	D	142	GLU	2.7
1	C	234	VAL	2.7
1	B	114	LEU	2.7
1	C	236	ALA	2.6
1	D	6	ARG	2.6
1	C	231	LEU	2.6
1	A	234	VAL	2.6
1	B	234	VAL	2.6
1	B	142	GLU	2.6
1	D	167	GLN	2.6
1	A	142	GLU	2.6
1	D	155	TYR	2.5
1	C	235	LEU	2.5
1	C	240	LEU	2.5
1	B	141	VAL	2.5
1	D	140	SER	2.4
1	D	70	HIS	2.4
1	B	96	GLN	2.4
1	D	277	VAL	2.3
1	A	106	THR	2.3
1	D	220	ARG	2.3
1	B	231	LEU	2.3
1	D	137	ARG	2.3
1	D	232	PRO	2.3
1	B	161	ARG	2.3
1	A	118	MET	2.2
1	C	70[A]	HIS	2.2
1	A	107	ASP	2.2
1	C	304	ILE	2.2
1	D	237	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	235	LEU	2.2
1	A	110	ALA	2.2
1	A	233	THR	2.1
1	C	286	HIS	2.1
1	C	303	ASP	2.1
1	D	238	LEU	2.1
1	C	110	ALA	2.1
1	B	145	ALA	2.1
1	D	160	GLU	2.1
1	D	202	ALA	2.1
1	A	284	VAL	2.1
1	D	148	ARG	2.0
1	A	302	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.