



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:38 PM UTC

PDB ID : 1GX3 / pdb_00001gx3
Title : M. smegmatis arylamine N-acetyl transferase
Authors : Sandy, J.; Mushtaq, A.; Kawamura, A.; Sinclair, J.; Sim, E.; Noble, M.
Deposited on : 2002-03-26
Resolution : 1.70 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

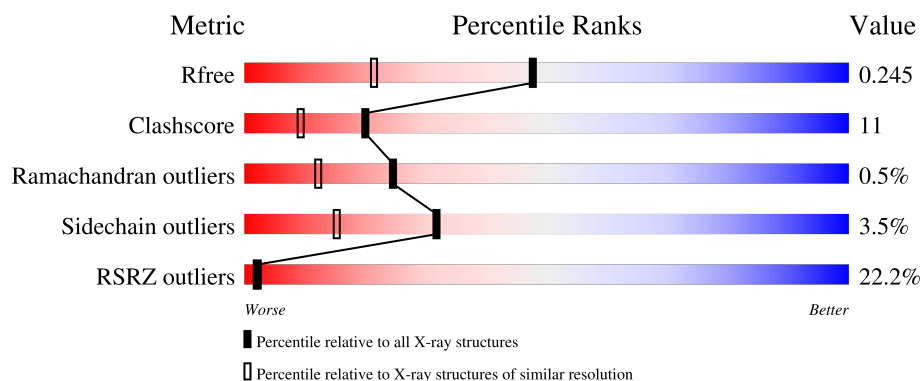
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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 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 $\leq 5\%$. 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	284	5% 87% 10% ..
1	B	284	15% 75% 19% ..
1	C	284	24% 73% 19% 5% .
1	D	284	42% 69% 25% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9263 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 ARYLAMINE N-ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2136	1339	395	398	4			
1	B	274	Total	C	N	O	S	0	0	0
			2124	1332	393	396	3			
1	C	274	Total	C	N	O	S	0	0	0
			2124	1332	393	396	3			
1	D	274	Total	C	N	O	S	0	0	0
			2124	1332	393	396	3			

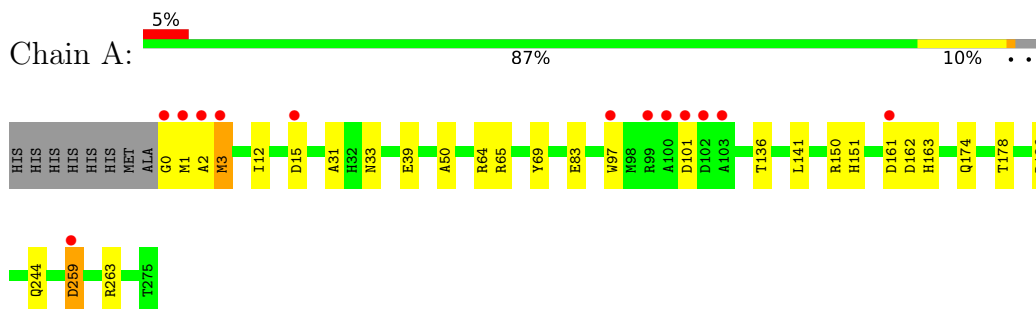
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	295	Total	O	0	0
			295	295		
2	B	218	Total	O	0	0
			218	218		
2	C	157	Total	O	0	0
			157	157		
2	D	85	Total	O	0	0
			85	85		

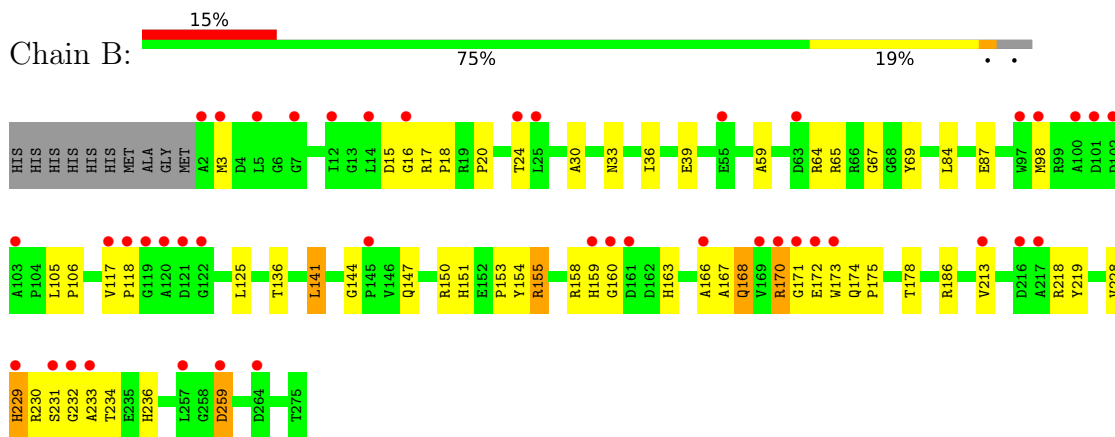
3 Residue-property plots [i](#)

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.

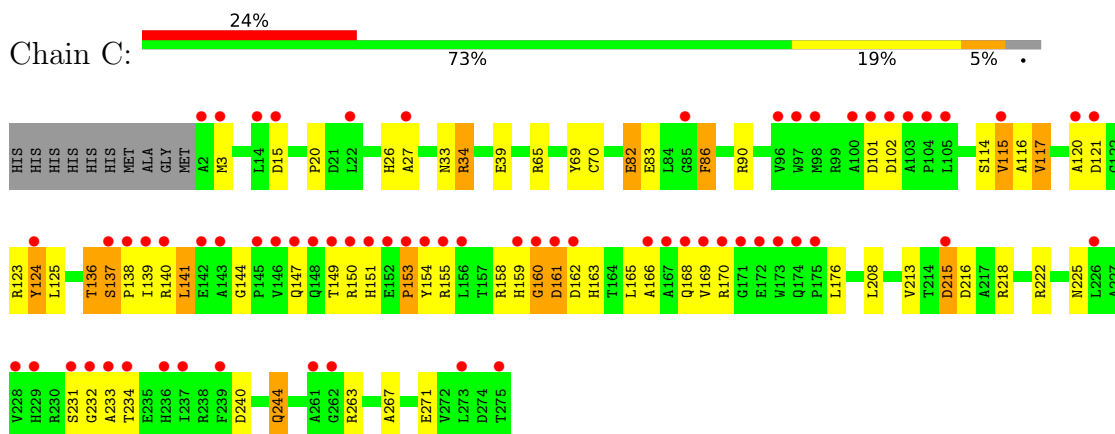
• Molecule 1: ARYLAMINE N-ACETYLTRANSFERASE



• Molecule 1: ARYLAMINE N-ACETYLTRANSFERASE



• Molecule 1: ARYLAMINE N-ACETYLTRANSFERASE



● Molecule 1: ARYLAMINE N-ACETYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.25Å 105.83Å 141.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 30.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-1.70) 97.8 (30.00-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.209 , 0.241 0.215 , 0.245	Depositor DCC
R_{free} test set	8181 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9263	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 3.22% 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

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	1.37	2/2184 (0.1%)	1.27	3/2974 (0.1%)
1	B	1.41	5/2172 (0.2%)	1.34	6/2959 (0.2%)
1	C	1.43	18/2172 (0.8%)	1.33	11/2959 (0.4%)
1	D	0.94	0/2172	1.11	6/2959 (0.2%)
All	All	1.30	25/8700 (0.3%)	1.26	26/11851 (0.2%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	116	ALA	CA-CB	-8.14	1.42	1.53
1	C	27	ALA	CA-CB	-6.96	1.42	1.53
1	C	153	PRO	C-O	6.56	1.31	1.23
1	B	175	PRO	C-O	6.46	1.31	1.23
1	C	82	GLU	CA-C	-6.42	1.44	1.52
1	C	137	SER	CA-CB	6.41	1.61	1.53
1	A	50	ALA	CA-CB	6.26	1.62	1.53
1	B	166	ALA	CA-C	6.22	1.60	1.52
1	C	215	ASP	CG-OD2	6.12	1.36	1.25
1	C	117	VAL	CA-C	6.07	1.59	1.52
1	C	123	ARG	C-O	5.84	1.31	1.23
1	C	26	HIS	CA-C	5.77	1.60	1.52
1	C	124	TYR	N-CA	-5.76	1.39	1.46
1	C	116	ALA	C-O	5.63	1.30	1.24
1	B	30	ALA	CA-CB	5.61	1.62	1.53
1	A	3	MET	SD-CE	-5.56	1.65	1.79
1	C	149	THR	CA-CB	-5.49	1.45	1.53
1	C	115	VAL	CA-C	5.46	1.59	1.52
1	B	174	GLN	CA-CB	-5.40	1.43	1.53
1	C	115	VAL	N-CA	-5.33	1.40	1.46
1	C	86	PHE	C-O	-5.32	1.16	1.23
1	C	138	PRO	CG-CD	-5.28	1.32	1.50
1	B	36	ILE	C-O	-5.12	1.18	1.23
1	C	166	ALA	C-O	-5.07	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	137	SER	C-N	-5.04	1.28	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	GLY	N-CA-C	10.60	127.12	113.24
1	A	101	ASP	N-CA-C	8.12	120.12	111.28
1	B	231	SER	CA-C-N	-7.02	111.36	120.14
1	B	231	SER	C-N-CA	-7.02	111.36	120.14
1	C	215	ASP	N-CA-C	-6.88	103.78	111.28
1	A	263	ARG	N-CA-C	6.27	121.09	113.38
1	D	225	ASN	N-CA-C	5.96	118.40	108.20
1	C	136	THR	CA-C-O	5.90	126.25	119.35
1	C	34	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	C	82	GLU	CB-CA-C	-5.78	101.81	110.88
1	A	161	ASP	N-CA-C	-5.76	106.01	113.16
1	D	138	PRO	N-CA-C	-5.73	102.12	111.68
1	C	215	ASP	CA-CB-CG	5.44	118.04	112.60
1	C	149	THR	CA-C-N	5.43	128.10	120.28
1	C	149	THR	C-N-CA	5.43	128.10	120.28
1	B	170	ARG	N-CA-C	-5.29	104.08	111.39
1	C	216	ASP	N-CA-C	5.27	120.72	113.97
1	D	213	VAL	CB-CA-C	-5.22	103.37	110.42
1	C	225	ASN	N-CA-C	5.21	117.22	108.73
1	C	70	CYS	N-CA-C	5.17	116.61	111.07
1	D	273	LEU	N-CA-C	5.16	116.59	111.07
1	D	88	VAL	N-CA-C	5.14	115.37	108.17
1	B	67	GLY	N-CA-C	-5.12	105.27	112.60
1	B	147	GLN	N-CA-C	5.07	117.23	109.07
1	D	67	GLY	N-CA-C	-5.04	105.66	112.57
1	C	114	SER	CA-C-O	5.03	125.68	120.30

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	2136	0	2095	29	1
1	B	2124	0	2080	45	0
1	C	2124	0	2080	55	1
1	D	2124	0	2080	65	0
2	A	295	0	0	16	1
2	B	218	0	0	23	0
2	C	157	0	0	13	1
2	D	85	0	0	12	0
All	All	9263	0	8335	192	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 11.

All (192) 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:A:15:ASP:HB2	2:A:2034:HOH:O	1.53	1.08
1:B:259:ASP:HB2	2:B:2205:HOH:O	1.61	1.01
1:A:97:TRP:CD2	2:A:2148:HOH:O	2.12	1.00
1:A:97:TRP:CE3	2:A:2148:HOH:O	2.12	1.00
1:D:241:SER:H	1:D:244:GLN:HE22	1.08	0.99
1:A:15:ASP:OD1	2:A:2035:HOH:O	1.81	0.98
1:D:259:ASP:HB3	2:D:2018:HOH:O	1.63	0.96
1:B:172:GLU:HA	2:B:2151:HOH:O	1.69	0.93
1:B:33:ASN:HD22	1:B:150:ARG:HH21	1.19	0.89
1:D:174:GLN:HG2	2:D:2057:HOH:O	1.73	0.89
1:D:241:SER:N	1:D:244:GLN:HE22	1.69	0.89
1:C:33:ASN:HD21	1:C:136:THR:HA	1.37	0.88
1:B:229:HIS:CD2	2:B:2194:HOH:O	2.27	0.88
1:C:101:ASP:HA	2:C:2077:HOH:O	1.73	0.87
1:B:98:MET:HG2	2:B:2086:HOH:O	1.72	0.87
1:B:118:PRO:HA	2:B:2099:HOH:O	1.76	0.86
1:D:18:PRO:HB3	1:D:24:THR:HG21	1.56	0.85
1:D:262:GLY:O	2:D:2082:HOH:O	1.92	0.85
1:A:33:ASN:HD22	1:A:150:ARG:HH21	1.26	0.84
1:B:228:VAL:O	2:B:2193:HOH:O	1.97	0.82
1:B:186:ARG:NH1	2:B:2163:HOH:O	2.09	0.82
1:C:121:ASP:OD1	2:C:2089:HOH:O	1.99	0.80
1:D:169:VAL:HB	1:D:174:GLN:NE2	1.96	0.80
1:D:259:ASP:CB	2:D:2018:HOH:O	2.27	0.79
1:B:170:ARG:NH2	1:B:233:ALA:O	2.16	0.78
1:C:215:ASP:HB2	2:C:2131:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLN:HG2	2:A:2215:HOH:O	1.84	0.77
1:D:262:GLY:C	2:D:2082:HOH:O	2.29	0.74
1:A:186:ARG:NH1	2:A:2225:HOH:O	2.21	0.73
1:B:155:ARG:NH2	2:B:2139:HOH:O	2.21	0.73
1:D:18:PRO:HB3	1:D:24:THR:CG2	2.18	0.72
1:D:56:ALA:O	2:D:2017:HOH:O	2.08	0.71
1:D:59:ALA:O	1:D:64:ARG:HG3	1.90	0.71
1:B:168:GLN:HG3	1:B:173:TRP:CE2	2.27	0.69
1:D:241:SER:H	1:D:244:GLN:NE2	1.85	0.69
1:B:172:GLU:HG2	2:B:2151:HOH:O	1.92	0.69
1:A:0:GLY:O	1:A:1:MET:HG2	1.93	0.69
1:C:150:ARG:N	2:C:2105:HOH:O	2.25	0.68
1:A:65:ARG:NH1	2:A:2107:HOH:O	2.15	0.68
1:D:17:ARG:HG2	1:D:17:ARG:HH11	1.58	0.67
1:D:260:LEU:HD22	1:D:263:ARG:HD2	1.76	0.67
1:D:161:ASP:OD1	1:D:180:THR:HB	1.95	0.67
1:A:97:TRP:CE2	2:A:2148:HOH:O	2.43	0.67
1:A:33:ASN:HD21	1:A:136:THR:HA	1.59	0.66
1:D:117:VAL:HB	1:D:120:ALA:HB3	1.76	0.66
1:C:153:PRO:HG2	1:C:168:GLN:NE2	2.13	0.64
1:A:1:MET:SD	2:A:2001:HOH:O	2.54	0.64
1:C:33:ASN:HD22	1:C:150:ARG:HH21	1.44	0.64
1:A:97:TRP:CZ3	2:A:2148:HOH:O	2.43	0.63
1:C:244:GLN:NE2	2:C:2141:HOH:O	2.32	0.62
1:D:87:GLU:HB3	1:D:116:ALA:HB3	1.82	0.62
1:A:65:ARG:NH2	2:A:2108:HOH:O	2.24	0.61
1:A:203:HIS:HE1	2:A:2246:HOH:O	1.83	0.60
1:D:174:GLN:CG	2:D:2057:HOH:O	2.38	0.60
1:B:33:ASN:HD21	1:B:136:THR:HA	1.65	0.60
1:A:203:HIS:HD2	2:A:2120:HOH:O	1.84	0.60
1:B:117:VAL:C	2:B:2097:HOH:O	2.44	0.60
1:C:144:GLY:O	1:C:155:ARG:NH1	2.34	0.60
1:C:33:ASN:ND2	1:C:136:THR:HA	2.15	0.59
1:B:172:GLU:CA	2:B:2151:HOH:O	2.37	0.59
1:C:240:ASP:H	1:C:244:GLN:NE2	2.01	0.58
1:A:33:ASN:HD22	1:A:150:ARG:NH2	1.97	0.58
1:C:139:ILE:HD11	1:C:165:LEU:CD1	2.34	0.57
1:C:140:ARG:HG3	1:C:147:GLN:OE1	2.04	0.57
1:B:144:GLY:O	1:B:155:ARG:HD2	2.04	0.57
1:D:3:MET:H	1:D:83:GLU:CD	2.13	0.57
1:D:4:ASP:O	1:D:5:LEU:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:THR:OG1	1:A:151:HIS:HD2	1.89	0.56
1:C:158:ARG:HD3	1:C:163:HIS:CE1	2.41	0.56
1:D:161:ASP:O	1:D:163:HIS:HD2	1.89	0.56
1:D:19:ARG:O	1:D:21:ASP:N	2.40	0.55
1:C:140:ARG:H	1:C:147:GLN:CD	2.14	0.55
1:B:98:MET:CG	2:B:2086:HOH:O	2.41	0.55
1:C:170:ARG:NH1	1:C:234:THR:OG1	2.40	0.54
1:C:136:THR:HG21	1:C:213:VAL:HG11	1.89	0.54
1:C:161:ASP:HB3	2:C:2111:HOH:O	2.08	0.53
1:C:215:ASP:OD1	2:C:2129:HOH:O	2.19	0.53
1:B:170:ARG:HH11	1:B:170:ARG:HG3	1.73	0.53
1:B:170:ARG:HE	1:B:234:THR:HG22	1.75	0.52
1:D:42:ASP:OD2	1:D:60:LYS:NZ	2.40	0.52
1:B:163:HIS:HE1	2:B:2120:HOH:O	1.91	0.52
1:B:236:HIS:HB3	2:B:2070:HOH:O	2.10	0.52
1:D:161:ASP:OD2	1:D:181:THR:OG1	2.27	0.52
1:D:174:GLN:CD	2:D:2057:HOH:O	2.54	0.51
1:B:154:TYR:CE2	1:B:167:ALA:HB2	2.45	0.51
1:C:140:ARG:N	1:C:147:GLN:OE1	2.36	0.50
1:B:17:ARG:NE	2:B:2010:HOH:O	2.36	0.50
1:B:159:HIS:CD2	2:B:2143:HOH:O	2.64	0.50
1:C:208:LEU:O	1:C:222:ARG:HD2	2.12	0.50
1:D:258:GLY:O	1:D:261:ALA:N	2.45	0.50
1:B:65:ARG:NH1	2:B:2059:HOH:O	2.18	0.50
1:C:20:PRO:HA	1:C:86:PHE:CZ	2.46	0.50
1:D:126:VAL:HG22	1:D:138:PRO:HB3	1.93	0.50
1:C:170:ARG:HH22	1:C:233:ALA:C	2.19	0.50
1:C:121:ASP:CG	2:C:2089:HOH:O	2.52	0.50
1:D:224:ARG:CZ	1:D:273:LEU:HD13	2.42	0.49
1:C:140:ARG:CB	1:C:147:GLN:OE1	2.60	0.49
1:D:262:GLY:C	2:D:2084:HOH:O	2.56	0.49
1:C:159:HIS:O	1:C:162:ASP:HB2	2.12	0.49
1:D:11:ARG:HD2	1:D:65:ARG:NH1	2.28	0.49
1:C:33:ASN:HD22	1:C:150:ARG:NH2	2.10	0.48
1:C:231:SER:HB2	2:C:2137:HOH:O	2.12	0.48
1:D:3:MET:HB2	1:D:83:GLU:HG2	1.94	0.48
1:D:224:ARG:NH1	1:D:273:LEU:HD13	2.28	0.48
1:D:24:THR:O	1:D:25:LEU:C	2.57	0.48
1:C:82:GLU:CD	1:C:90:ARG:HH12	2.21	0.48
1:C:153:PRO:HB2	1:C:168:GLN:CG	2.43	0.48
1:B:213:VAL:HG13	1:B:218:ARG:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:VAL:HB	1:C:120:ALA:HB3	1.96	0.48
1:B:16:GLY:O	1:B:18:PRO:HD3	2.15	0.47
1:C:153:PRO:HD2	1:C:168:GLN:HG3	1.95	0.47
1:D:122:GLY:N	2:D:2039:HOH:O	2.48	0.47
1:C:153:PRO:HB2	1:C:168:GLN:HE21	1.78	0.47
1:B:136:THR:HG21	1:B:151:HIS:CD2	2.49	0.47
1:D:116:ALA:O	1:D:118:PRO:HD3	2.14	0.47
1:C:140:ARG:HB2	1:C:147:GLN:OE1	2.15	0.46
1:A:1:MET:HG3	1:A:2:ALA:N	2.29	0.46
1:C:125:LEU:HB2	1:C:141:LEU:HD22	1.97	0.46
1:D:220:ASN:HB2	2:D:2077:HOH:O	2.14	0.46
1:C:125:LEU:HD23	1:C:165:LEU:HD13	1.98	0.46
1:C:263:ARG:NH1	2:C:2150:HOH:O	2.49	0.46
1:D:17:ARG:HG2	1:D:17:ARG:NH1	2.27	0.46
1:C:136:THR:CG2	1:C:213:VAL:HG11	2.46	0.46
1:D:22:LEU:O	1:D:23:GLY:C	2.56	0.46
1:D:146:VAL:HG22	1:D:155:ARG:HD3	1.97	0.46
1:B:17:ARG:O	1:B:17:ARG:CG	2.63	0.46
1:A:136:THR:OG1	1:A:151:HIS:CD2	2.69	0.45
1:B:153:PRO:HG2	1:B:168:GLN:NE2	2.31	0.45
1:B:168:GLN:HG3	1:B:173:TRP:CD2	2.52	0.45
1:C:232:GLY:O	1:D:240:ASP:N	2.49	0.45
1:B:158:ARG:NE	2:B:2144:HOH:O	2.40	0.45
1:D:45:LEU:HD23	1:D:268:ARG:HG2	1.97	0.45
1:B:163:HIS:O	1:B:178:THR:HA	2.17	0.45
1:D:208:LEU:O	1:D:222:ARG:HD2	2.17	0.45
1:A:64:ARG:NH2	2:A:2105:HOH:O	2.50	0.44
1:B:118:PRO:N	2:B:2097:HOH:O	2.50	0.44
1:B:125:LEU:HB2	1:B:141:LEU:CD2	2.48	0.44
1:C:115:VAL:O	1:C:124:TYR:N	2.39	0.44
1:A:259:ASP:OD1	1:A:259:ASP:C	2.60	0.44
1:D:136:THR:OG1	1:D:151:HIS:HD2	2.00	0.44
1:C:151:HIS:HB2	1:C:218:ARG:HH21	1.81	0.44
1:D:260:LEU:CD2	1:D:263:ARG:HD2	2.45	0.44
1:D:18:PRO:CB	1:D:24:THR:HG21	2.38	0.44
1:A:163:HIS:O	1:A:178:THR:HA	2.18	0.44
1:C:153:PRO:HB2	1:C:168:GLN:HG2	2.00	0.44
1:C:218:ARG:NH2	2:C:2132:HOH:O	2.50	0.44
1:D:158:ARG:HH11	1:D:158:ARG:HG2	1.83	0.44
1:B:171:GLY:C	2:B:2151:HOH:O	2.60	0.43
1:C:161:ASP:O	1:C:163:HIS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:VAL:HB	1:D:174:GLN:HE22	1.78	0.43
1:D:218:ARG:HB2	1:D:229:HIS:HB2	2.00	0.43
1:C:15:ASP:O	1:C:15:ASP:OD1	2.35	0.43
1:D:241:SER:CA	1:D:244:GLN:HE22	2.29	0.43
1:B:219:TYR:CE2	1:B:228:VAL:HG13	2.53	0.43
1:D:263:ARG:HD3	2:D:2083:HOH:O	2.19	0.43
1:C:267:ALA:O	1:C:271:GLU:HG3	2.19	0.43
1:D:74:ASN:O	1:D:113:LEU:HD21	2.19	0.43
1:B:153:PRO:HG2	1:B:168:GLN:HE21	1.84	0.43
1:B:259:ASP:CB	2:B:2205:HOH:O	2.38	0.42
1:B:144:GLY:C	2:B:2125:HOH:O	2.62	0.42
1:D:161:ASP:O	1:D:163:HIS:CD2	2.69	0.42
1:D:3:MET:HE3	1:D:83:GLU:HB2	2.01	0.42
1:D:163:HIS:O	1:D:178:THR:HA	2.19	0.42
1:A:3:MET:HE2	1:A:83:GLU:HG2	2.02	0.42
1:C:160:GLY:C	1:C:162:ASP:H	2.28	0.42
1:D:245:VAL:O	1:D:246:LEU:C	2.59	0.42
1:D:54:ALA:O	1:D:55:GLU:C	2.63	0.42
1:A:33:ASN:ND2	1:A:150:ARG:HH21	2.04	0.41
1:B:20:PRO:HG3	1:B:84:LEU:O	2.20	0.41
1:C:240:ASP:HB2	1:C:244:GLN:HE22	1.85	0.41
1:A:174:GLN:CG	2:A:2215:HOH:O	2.54	0.41
1:B:105:LEU:HA	1:B:106:PRO:HD3	1.90	0.41
1:D:143:ALA:HA	1:D:156:LEU:O	2.20	0.41
1:A:0:GLY:O	1:A:1:MET:CG	2.66	0.41
1:B:159:HIS:O	1:B:160:GLY:C	2.61	0.41
1:C:101:ASP:O	1:C:102:ASP:HB2	2.20	0.41
1:C:154:TYR:HE2	1:C:176:LEU:HD11	1.84	0.41
1:D:39:GLU:HG2	1:D:67:GLY:HA3	2.03	0.41
1:C:150:ARG:CG	2:C:2105:HOH:O	2.68	0.41
1:D:42:ASP:HB2	1:D:43:PRO:HD3	2.03	0.41
1:C:232:GLY:O	1:D:240:ASP:HB2	2.20	0.41
1:A:97:TRP:HZ3	2:A:2083:HOH:O	2.03	0.40
1:B:59:ALA:O	1:B:64:ARG:HG3	2.21	0.40
1:C:140:ARG:CG	1:C:147:GLN:OE1	2.68	0.40
1:A:12:ILE:O	1:A:31:ALA:HB1	2.21	0.40
1:C:3:MET:HB3	1:C:83:GLU:HG2	2.02	0.40
1:B:236:HIS:CB	2:B:2070:HOH:O	2.69	0.40
1:C:150:ARG:CA	2:C:2105:HOH:O	2.68	0.40
1:D:41:LEU:HB2	1:D:66:ARG:NH1	2.36	0.40
1:D:153:PRO:HG2	1:D:168:GLN:HE21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:LEU:N	1:D:176:LEU:HD23	2.36	0.40
1:D:244:GLN:HE21	1:D:244:GLN:HB2	1.56	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ASP:OD2	1:C:34:ARG:NH1[3_545]	2.12	0.08
2:A:2029:HOH:O	2:C:2006:HOH:O[3_545]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	274/284 (96%)	264 (96%)	10 (4%)	0	100	100
1	B	272/284 (96%)	261 (96%)	10 (4%)	1 (0%)	30	16
1	C	272/284 (96%)	262 (96%)	8 (3%)	2 (1%)	18	7
1	D	272/284 (96%)	246 (90%)	24 (9%)	2 (1%)	18	7
All	All	1090/1136 (96%)	1033 (95%)	52 (5%)	5 (0%)	24	12

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	18	PRO
1	B	3	MET
1	C	160	GLY
1	D	20	PRO
1	C	161	ASP

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	221/228 (97%)	215 (97%)	6 (3%)	39	23
1	B	220/228 (96%)	209 (95%)	11 (5%)	22	8
1	C	220/228 (96%)	213 (97%)	7 (3%)	34	17
1	D	220/228 (96%)	213 (97%)	7 (3%)	34	17
All	All	881/912 (97%)	850 (96%)	31 (4%)	32	15

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	69	TYR
1	A	141	LEU
1	A	162	ASP
1	A	244	GLN
1	A	259	ASP
1	B	15	ASP
1	B	24	THR
1	B	39	GLU
1	B	69	TYR
1	B	87	GLU
1	B	141	LEU
1	B	155	ARG
1	B	168	GLN
1	B	229	HIS
1	B	230	ARG
1	B	259	ASP
1	C	39	GLU
1	C	65	ARG
1	C	69	TYR
1	C	137	SER
1	C	141	LEU
1	C	169	VAL
1	C	244	GLN

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Mol	Chain	Res	Type
1	D	24	THR
1	D	39	GLU
1	D	69	TYR
1	D	141	LEU
1	D	176	LEU
1	D	240	ASP
1	D	244	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	133	GLN
1	A	148	GLN
1	A	151	HIS
1	A	168	GLN
1	A	203	HIS
1	A	225	ASN
1	A	229	HIS
1	A	244	GLN
1	B	33	ASN
1	B	133	GLN
1	B	148	GLN
1	B	151	HIS
1	B	168	GLN
1	B	220	ASN
1	B	225	ASN
1	B	236	HIS
1	B	244	GLN
1	B	251	ASN
1	C	33	ASN
1	C	151	HIS
1	C	163	HIS
1	C	168	GLN
1	C	220	ASN
1	C	225	ASN
1	C	244	GLN
1	D	33	ASN
1	D	133	GLN
1	D	151	HIS
1	D	163	HIS
1	D	168	GLN

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Mol	Chain	Res	Type
1	D	174	GLN
1	D	220	ASN
1	D	244	GLN
1	D	251	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 oligosaccharides 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

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, 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	276/284 (97%)	0.28	14 (5%) 33 37	18, 26, 47, 68	0
1	B	274/284 (96%)	0.98	43 (15%) 5 4	20, 32, 54, 65	0
1	C	274/284 (96%)	1.16	67 (24%) 2 2	21, 35, 58, 69	0
1	D	274/284 (96%)	1.90	120 (43%) 0 0	28, 51, 73, 82	0
All	All	1098/1136 (96%)	1.08	244 (22%) 2 2	18, 35, 63, 82	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	261	ALA	6.4
1	D	100	ALA	5.9
1	A	1	MET	5.8
1	B	119	GLY	5.5
1	B	120	ALA	5.4
1	C	146	VAL	5.4
1	B	118	PRO	5.3
1	D	262	GLY	5.2
1	D	16	GLY	4.9
1	D	14	LEU	4.8
1	D	257	LEU	4.8
1	B	159	HIS	4.7
1	D	2	ALA	4.6
1	C	153	PRO	4.6
1	A	97	TRP	4.5
1	B	259	ASP	4.4
1	C	103	ALA	4.4
1	C	173	TRP	4.4
1	C	232	GLY	4.4
1	D	22	LEU	4.4
1	A	102	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	259	ASP	4.4
1	B	101	ASP	4.4
1	D	117	VAL	4.3
1	C	148	GLN	4.3
1	D	97	TRP	4.2
1	D	28	ILE	4.2
1	B	160	GLY	4.1
1	D	5	LEU	4.1
1	D	146	VAL	4.1
1	D	273	LEU	4.1
1	D	19	ARG	4.1
1	C	262	GLY	4.0
1	D	245	VAL	4.0
1	C	97	TRP	4.0
1	B	2	ALA	4.0
1	D	233	ALA	4.0
1	D	12	ILE	3.9
1	A	161	ASP	3.9
1	B	121	ASP	3.9
1	C	171	GLY	3.9
1	D	119	GLY	3.9
1	D	242	ALA	3.9
1	C	169	VAL	3.8
1	D	98	MET	3.8
1	C	100	ALA	3.8
1	D	120	ALA	3.7
1	D	243	ALA	3.7
1	D	102	ASP	3.7
1	D	260	LEU	3.7
1	D	275	THR	3.7
1	C	2	ALA	3.7
1	D	141	LEU	3.7
1	B	102	ASP	3.7
1	B	117	VAL	3.6
1	D	259	ASP	3.6
1	B	161	ASP	3.6
1	C	145	PRO	3.6
1	B	166	ALA	3.6
1	C	102	ASP	3.6
1	D	118	PRO	3.6
1	C	170	ARG	3.5
1	D	231	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	151	HIS	3.5
1	C	159	HIS	3.5
1	D	3	MET	3.5
1	C	228	VAL	3.5
1	D	124	TYR	3.5
1	C	160	GLY	3.5
1	D	103	ALA	3.4
1	D	246	LEU	3.4
1	C	101	ASP	3.4
1	D	148	GLN	3.4
1	D	269	VAL	3.3
1	B	3	MET	3.3
1	A	2	ALA	3.3
1	D	116	ALA	3.3
1	B	172	GLU	3.3
1	A	101	ASP	3.3
1	D	54	ALA	3.3
1	C	154	TYR	3.2
1	C	104	PRO	3.2
1	D	173	TRP	3.2
1	D	61	LEU	3.2
1	C	167	ALA	3.2
1	D	23	GLY	3.2
1	D	139	ILE	3.2
1	A	0	GLY	3.2
1	C	143	ALA	3.2
1	D	27	ALA	3.2
1	C	161	ASP	3.1
1	C	137	SER	3.1
1	B	264	ASP	3.1
1	D	62	VAL	3.1
1	C	172	GLU	3.1
1	D	47	ILE	3.1
1	B	14	LEU	3.1
1	C	233	ALA	3.1
1	B	24	THR	3.1
1	C	239	PHE	3.1
1	B	170	ARG	3.0
1	D	149	THR	3.0
1	A	100	ALA	3.0
1	D	9	LEU	3.0
1	D	232	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	239	PHE	3.0
1	C	121	ASP	2.9
1	C	149	THR	2.9
1	B	217	ALA	2.9
1	A	15	ASP	2.9
1	B	98	MET	2.9
1	C	234	THR	2.9
1	D	156	LEU	2.9
1	C	139	ILE	2.9
1	D	88	VAL	2.9
1	D	265	VAL	2.9
1	D	4	ASP	2.9
1	A	103	ALA	2.8
1	B	233	ALA	2.8
1	C	226	LEU	2.8
1	D	20	PRO	2.8
1	D	25	LEU	2.8
1	D	101	ASP	2.8
1	D	240	ASP	2.8
1	D	247	ASP	2.8
1	B	122	GLY	2.8
1	D	59	ALA	2.8
1	D	270	ALA	2.8
1	B	25	LEU	2.8
1	B	232	GLY	2.8
1	B	173	TRP	2.7
1	C	138	PRO	2.7
1	D	18	PRO	2.7
1	D	237	ILE	2.7
1	D	136	THR	2.7
1	D	244	GLN	2.7
1	C	175	PRO	2.7
1	D	15	ASP	2.7
1	C	124	TYR	2.7
1	B	100	ALA	2.7
1	D	17	ARG	2.7
1	B	97	TRP	2.7
1	C	156	LEU	2.7
1	D	29	VAL	2.7
1	D	250	VAL	2.7
1	C	120	ALA	2.7
1	D	31	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	174	GLN	2.6
1	D	24	THR	2.6
1	B	169	VAL	2.6
1	D	115	VAL	2.6
1	D	154	TYR	2.6
1	C	155	ARG	2.6
1	D	264	ASP	2.6
1	D	56	ALA	2.6
1	B	257	LEU	2.6
1	D	87	GLU	2.6
1	D	86	PHE	2.5
1	D	272	VAL	2.5
1	B	171	GLY	2.5
1	D	81	LEU	2.5
1	C	162	ASP	2.5
1	C	168	GLN	2.5
1	C	85	GLY	2.5
1	D	45	LEU	2.5
1	C	166	ALA	2.5
1	D	50	ALA	2.5
1	B	12	ILE	2.5
1	C	236	HIS	2.5
1	C	275	THR	2.5
1	D	174	GLN	2.4
1	D	76	LEU	2.4
1	B	16	GLY	2.4
1	D	80	VAL	2.4
1	D	249	ILE	2.4
1	A	3	MET	2.4
1	A	232	GLY	2.4
1	C	14	LEU	2.4
1	C	273	LEU	2.4
1	B	231	SER	2.4
1	D	159	HIS	2.4
1	C	231	SER	2.4
1	D	63	ASP	2.4
1	D	183	PRO	2.3
1	B	55	GLU	2.3
1	C	150	ARG	2.3
1	D	234	THR	2.3
1	D	274	ASP	2.3
1	D	255	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	21	ASP	2.3
1	B	103	ALA	2.3
1	D	57	LEU	2.3
1	D	122	GLY	2.3
1	B	145	PRO	2.3
1	D	241	SER	2.3
1	D	162	ASP	2.3
1	D	258	GLY	2.3
1	C	96	VAL	2.3
1	C	229	HIS	2.2
1	D	10	THR	2.2
1	D	13	GLY	2.2
1	D	79	TYR	2.2
1	D	155	ARG	2.2
1	D	143	ALA	2.2
1	C	15	ASP	2.2
1	C	152	GLU	2.2
1	D	214	THR	2.2
1	C	115	VAL	2.2
1	B	63	ASP	2.2
1	D	83	GLU	2.2
1	B	7	GLY	2.2
1	C	22	LEU	2.2
1	C	105	LEU	2.2
1	D	84	LEU	2.2
1	C	140	ARG	2.2
1	C	237	ILE	2.2
1	C	3	MET	2.1
1	C	215	ASP	2.1
1	C	147	GLN	2.1
1	D	248	ALA	2.1
1	D	32	HIS	2.1
1	D	216	ASP	2.1
1	D	64	ARG	2.1
1	B	213	VAL	2.1
1	D	30	ALA	2.1
1	B	5	LEU	2.1
1	D	77	LEU	2.1
1	C	98	MET	2.1
1	B	216	ASP	2.1
1	A	99	ARG	2.1
1	D	267	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	225	ASN	2.1
1	D	251	ASN	2.1
1	D	52	LEU	2.1
1	D	65	ARG	2.1
1	D	170	ARG	2.1
1	D	157	THR	2.1
1	D	206	THR	2.1
1	C	27	ALA	2.0
1	C	142	GLU	2.0
1	C	261	ALA	2.0
1	D	58	PHE	2.0
1	D	150	ARG	2.0
1	B	229	HIS	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 oligosaccharides 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.