



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:43 am BST

PDB ID : 1GX3
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 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

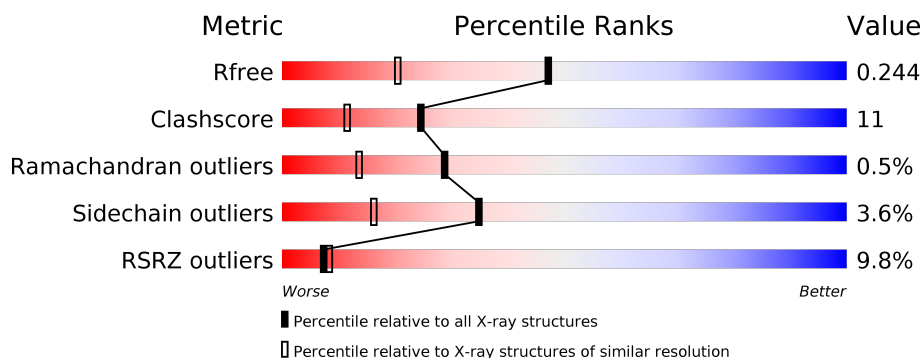
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 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	284	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>• •</div> </div> </div>
1	B	284	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• • •</div> </div> </div>
1	C	284	<div> <div>9%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>• •</div> </div> </div>
1	D	284	<div> <div>21%</div> <div> <div></div> <div>68%</div> <div>25%</div> <div>• •</div> </div> </div>

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.

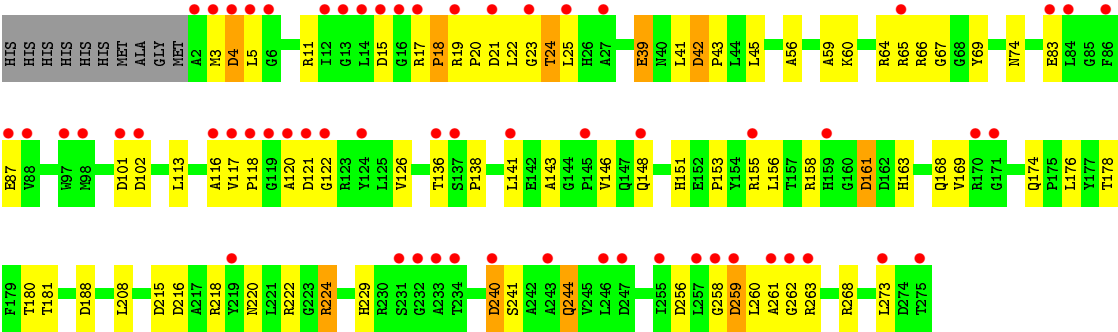
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2136	1339	395	398	4			
1	B	274	Total	C	N	O	S	0	0	0
			2124	1332	393	396	3			
1	C	274	Total	C	N	O	S	0	0	0
			2124	1332	393	396	3			
1	D	274	Total	C	N	O	S	0	0	0
			2124	1332	393	396	3			

- 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		

● 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 84.71 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-1.70) 97.8 (84.71-1.70)	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 , 0.244	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)	0.36 , 47.6	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	1.13	3/2184 (0.1%)	1.21	17/2974 (0.6%)
1	B	1.13	4/2172 (0.2%)	1.17	17/2959 (0.6%)
1	C	1.12	8/2172 (0.4%)	1.17	13/2959 (0.4%)
1	D	0.73	0/2172	0.96	12/2959 (0.4%)
All	All	1.04	15/8700 (0.2%)	1.13	59/11851 (0.5%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	172	GLU	CD-OE1	6.43	1.32	1.25
1	B	29	VAL	CB-CG1	6.30	1.66	1.52
1	C	29	VAL	CB-CG1	-5.98	1.40	1.52
1	C	137	SER	CA-CB	5.83	1.61	1.52
1	B	112	VAL	CB-CG2	-5.63	1.41	1.52
1	A	55	GLU	CD-OE1	5.59	1.31	1.25
1	C	215	ASP	CB-CG	5.50	1.63	1.51
1	C	138	PRO	CG-CD	-5.41	1.32	1.50
1	C	69	TYR	CD2-CE2	5.41	1.47	1.39
1	A	8	TYR	CE1-CZ	-5.27	1.31	1.38
1	B	146	VAL	CB-CG1	-5.24	1.41	1.52
1	C	124	TYR	CB-CG	5.23	1.59	1.51
1	C	124	TYR	CD1-CE1	5.21	1.47	1.39
1	C	215	ASP	CG-OD2	5.06	1.36	1.25
1	A	69	TYR	CD2-CE2	5.02	1.46	1.39

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	ASP	CB-CG-OD2	9.96	127.26	118.30
1	A	64	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	D	188	ASP	CB-CG-OD2	9.06	126.45	118.30
1	C	4	ASP	CB-CG-OD2	8.56	126.00	118.30
1	A	64	ARG	NE-CZ-NH1	8.53	124.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	34	ARG	NE-CZ-NH2	8.38	124.49	120.30
1	B	256	ASP	CB-CG-OD2	8.35	125.81	118.30
1	B	155	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	C	21	ASP	CB-CG-OD2	7.53	125.08	118.30
1	C	274	ASP	CB-CG-OD2	7.45	125.01	118.30
1	B	155	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	218	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	101	ASP	CB-CG-OD2	7.15	124.73	118.30
1	A	162	ASP	CB-CG-OD2	7.09	124.68	118.30
1	D	161	ASP	CB-CG-OD2	6.88	124.49	118.30
1	B	101	ASP	CB-CG-OD2	6.83	124.44	118.30
1	C	264	ASP	CB-CG-OD2	6.75	124.38	118.30
1	A	215	ASP	CB-CG-OD1	6.55	124.19	118.30
1	B	274	ASP	CB-CG-OD2	6.32	123.99	118.30
1	A	150	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	D	259	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	165	LEU	CB-CG-CD1	-6.02	100.77	111.00
1	A	141	LEU	CB-CG-CD1	5.98	121.17	111.00
1	C	15	ASP	CB-CG-OD2	5.96	123.67	118.30
1	C	34	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	C	90	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	121	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	230	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	D	4	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	69	TYR	CB-CG-CD2	5.75	124.45	121.00
1	B	63	ASP	CB-CG-OD2	5.70	123.43	118.30
1	D	256	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	238	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	232	GLY	N-CA-C	5.61	127.12	113.10
1	D	215	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	216	ASP	CB-CG-OD2	5.56	123.30	118.30
1	D	15	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	64	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	D	216	ASP	CB-CG-OD2	5.53	123.28	118.30
1	D	101	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	268	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	D	121	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	162	ASP	CB-CG-OD2	5.46	123.22	118.30
1	D	102	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	259	ASP	OD1-CG-OD2	-5.41	113.02	123.30
1	C	161	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	102	ASP	CB-CG-OD2	5.34	123.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	ASP	CB-CG-OD2	5.25	123.03	118.30
1	C	125	LEU	CB-CG-CD2	5.24	119.91	111.00
1	B	170	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	231	SER	C-N-CA	-5.21	111.36	122.30
1	B	172	GLU	OE1-CD-OE2	5.18	129.52	123.30
1	A	17	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	102	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	268	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	D	42	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	63	ASP	CB-CG-OD2	5.03	122.82	118.30
1	B	170	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	B	141	LEU	CB-CG-CD1	5.00	119.51	111.00

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	27	1
1	B	2124	0	2080	42	0
1	C	2124	0	2080	54	1
1	D	2124	0	2080	62	0
2	A	295	0	0	16	1
2	B	218	0	0	21	0
2	C	157	0	0	13	1
2	D	85	0	0	12	0
All	All	9263	0	8335	183	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 (183) 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
1:A:174:GLN:HG2	2:A:2215:HOH:O	1.84	0.77
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:D:262:GLY:C	2:D:2082:HOH:O	2.29	0.69
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:HH11	1:D:17:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:4:ASP:O	1:D:5:LEU:HB2	2.05	0.57
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:B:117:VAL:C	2:B:2097:HOH:O	2.44	0.55
1:D:19:ARG:O	1:D:21:ASP:N	2.40	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:3:MET:H	1:D:83:GLU:CD	2.13	0.52
1:B:154:TYR:CE2	1:B:167:ALA:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:140:ARG:H	1:C:147:GLN:CD	2.14	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: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: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:224:ARG:NH1	1:D:273:LEU:HD13	2.28	0.48
1:D:3:MET:HB2	1:D:83:GLU:HG2	1.94	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
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:174:GLN:CD	2:D:2057:HOH:O	2.54	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:NH1	1:D:17:ARG:HG2	2.27	0.46
1:C:136:THR:CG2	1:C:213:VAL:HG11	2.46	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:C:170:ARG:HH22	1:C:233:ALA:C	2.19	0.45
1:B:168:GLN:HG3	1:B:173:TRP:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:262:GLY:C	2:D:2084:HOH:O	2.56	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:C:161:ASP:O	1:C:163:HIS:HD2	2.01	0.43
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:82:GLU:CD	1:C:90:ARG:HH12	2.21	0.43
1:D:24:THR:O	1:D:25:LEU:C	2.57	0.43
1:C:15:ASP:OD1	1:C:15:ASP:O	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:D:161:ASP:O	1:D:163:HIS:CD2	2.69	0.42
1:D:163:HIS:O	1:D:178:THR:HA	2.19	0.42
1:C:121:ASP:CG	2:C:2089:HOH:O	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:LEU:O	1:D:23:GLY:C	2.56	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:153:PRO:HG2	1:D:168:GLN:HE21	1.87	0.40
1:D:176:LEU:N	1:D:176:LEU:HD23	2.36	0.40
1:D:41:LEU:HB2	1:D:66:ARG:NH1	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	274/284 (96%)	264 (96%)	10 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	272/284 (96%)	261 (96%)	10 (4%)	1 (0%)	34	18
1	C	272/284 (96%)	262 (96%)	8 (3%)	2 (1%)	22	8
1	D	272/284 (96%)	246 (90%)	24 (9%)	2 (1%)	22	8
All	All	1090/1136 (96%)	1033 (95%)	52 (5%)	5 (0%)	29	13

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%)	214 (97%)	7 (3%)	39	20
1	B	220/228 (96%)	210 (96%)	10 (4%)	27	10
1	C	220/228 (96%)	213 (97%)	7 (3%)	39	20
1	D	220/228 (96%)	212 (96%)	8 (4%)	35	16
All	All	881/912 (97%)	849 (96%)	32 (4%)	35	16

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	39	GLU
1	A	69	TYR
1	A	141	LEU
1	A	162	ASP
1	A	244	GLN

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Mol	Chain	Res	Type
1	A	259	ASP
1	B	15	ASP
1	B	17	ARG
1	B	39	GLU
1	B	69	TYR
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	97	TRP
1	C	137	SER
1	C	141	LEU
1	C	244	GLN
1	D	24	THR
1	D	39	GLU
1	D	69	TYR
1	D	141	LEU
1	D	148	GLN
1	D	224	ARG
1	D	240	ASP
1	D	244	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	151	HIS
1	A	168	GLN
1	A	203	HIS
1	A	229	HIS
1	A	244	GLN
1	A	251	ASN
1	B	33	ASN
1	B	108	GLN
1	B	148	GLN
1	B	151	HIS
1	B	159	HIS

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Mol	Chain	Res	Type
1	B	168	GLN
1	B	244	GLN
1	B	251	ASN
1	C	33	ASN
1	C	108	GLN
1	C	151	HIS
1	C	163	HIS
1	C	168	GLN
1	C	244	GLN
1	D	33	ASN
1	D	151	HIS
1	D	163	HIS
1	D	168	GLN
1	D	174	GLN
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 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

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%)	0.37	6 (2%) 62 66	18, 26, 47, 68	0
1	B	274/284 (96%)	0.49	16 (5%) 23 25	20, 32, 54, 65	0
1	C	274/284 (96%)	0.56	25 (9%) 9 10	21, 35, 58, 69	0
1	D	274/284 (96%)	1.21	61 (22%) 0 0	28, 51, 73, 82	0
All	All	1098/1136 (96%)	0.66	108 (9%) 7 8	18, 35, 63, 82	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	8.5
1	D	119	GLY	7.3
1	D	3	MET	7.2
1	D	233	ALA	7.1
1	D	117	VAL	6.8
1	D	261	ALA	6.5
1	A	0	GLY	6.3
1	B	119	GLY	6.3
1	D	16	GLY	6.1
1	D	15	ASP	5.9
1	D	102	ASP	5.9
1	D	262	GLY	5.8
1	D	14	LEU	5.5
1	D	232	GLY	5.3
1	D	120	ALA	5.3
1	C	232	GLY	5.2
1	D	2	ALA	5.1
1	D	4	ASP	5.0
1	D	19	ARG	4.9
1	B	101	ASP	4.9
1	A	102	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	118	PRO	4.8
1	D	23	GLY	4.8
1	C	102	ASP	4.7
1	C	262	GLY	4.6
1	C	170	ARG	4.4
1	C	169	VAL	4.3
1	D	118	PRO	4.1
1	D	259	ASP	4.1
1	D	257	LEU	3.9
1	B	121	ASP	3.9
1	D	148	GLN	3.9
1	D	275	THR	3.9
1	C	171	GLY	3.8
1	D	17	ARG	3.8
1	D	121	ASP	3.8
1	B	120	ALA	3.8
1	B	160	GLY	3.8
1	D	124	TYR	3.8
1	A	101	ASP	3.8
1	C	101	ASP	3.8
1	B	102	ASP	3.7
1	D	27	ALA	3.7
1	C	2	ALA	3.6
1	B	16	GLY	3.6
1	B	159	HIS	3.5
1	C	148	GLN	3.5
1	D	159	HIS	3.5
1	D	122	GLY	3.4
1	C	15	ASP	3.4
1	B	259	ASP	3.4
1	D	171	GLY	3.3
1	D	155	ARG	3.2
1	D	170	ARG	3.2
1	D	5	LEU	3.2
1	C	97	TRP	3.1
1	D	97	TRP	3.0
1	C	159	HIS	3.0
1	D	65	ARG	2.9
1	D	6	GLY	2.9
1	D	12	ILE	2.9
1	A	161	ASP	2.9
1	B	161	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	101	ASP	2.8
1	C	231	SER	2.8
1	D	258	GLY	2.7
1	C	153	PRO	2.7
1	D	83	GLU	2.7
1	B	2	ALA	2.7
1	C	174	GLN	2.7
1	A	97	TRP	2.7
1	D	246	LEU	2.7
1	B	117	VAL	2.7
1	D	136	THR	2.6
1	C	161	ASP	2.6
1	D	88	VAL	2.6
1	C	103	ALA	2.5
1	D	263	ARG	2.5
1	D	84	LEU	2.5
1	D	231	SER	2.5
1	C	172	GLU	2.5
1	D	98	MET	2.4
1	D	87	GLU	2.4
1	D	25	LEU	2.4
1	B	15	ASP	2.4
1	C	173	TRP	2.4
1	D	273	LEU	2.4
1	C	160	GLY	2.4
1	D	86	PHE	2.4
1	D	240	ASP	2.4
1	D	234	THR	2.4
1	D	21	ASP	2.3
1	B	264	ASP	2.3
1	D	137	SER	2.3
1	C	104	PRO	2.2
1	C	100	ALA	2.2
1	D	13	GLY	2.2
1	D	219	TYR	2.1
1	D	145	PRO	2.1
1	C	121	ASP	2.1
1	C	239	PHE	2.1
1	D	116	ALA	2.1
1	D	141	LEU	2.1
1	C	233	ALA	2.0
1	D	243	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	255	ILE	2.0
1	D	247	ASP	2.0
1	B	98	MET	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.