



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 12:00 pm GMT

PDB ID : 1W6F  
Title : Arylamine N-acetyltransferase from Mycobacterium smegmatis with the anti-tubercular drug isoniazid bound in the active site.  
Authors : Sandy, J.; Holton, S.; Fullham, E.; Sim, E.; Noble, M.E.M.  
Deposited on : 2004-08-17  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

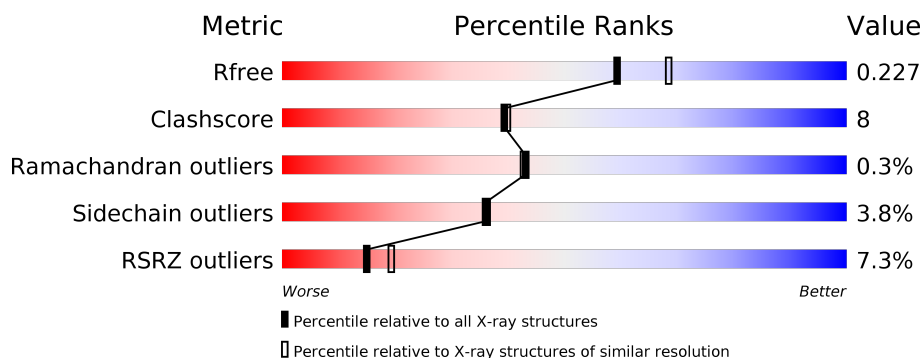
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	278	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>••</div> </div> </div>
1	B	278	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>•</div> </div> </div>
1	C	278	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>••</div> </div> </div>
1	D	278	<div> <div>13%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>••</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ISZ	A	1276	-	-	X	-

## 2 Entry composition [i](#)

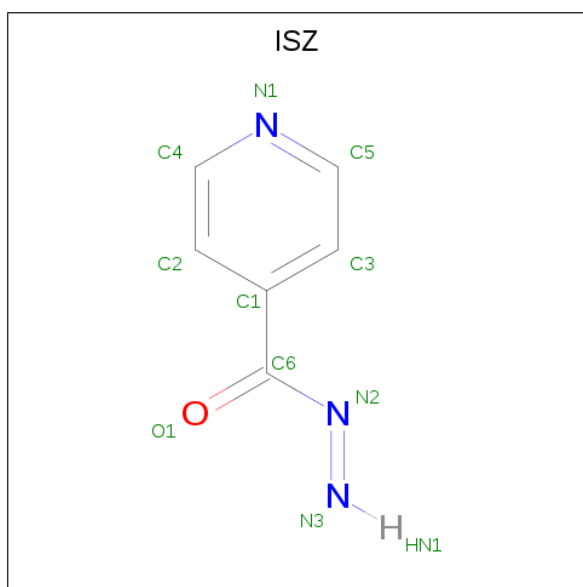
There are 3 unique types of molecules in this entry. The entry contains 9166 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	273	Total	C	N	O	S	0	0	0
			2119	1329	392	395	3			
1	B	269	Total	C	N	O	S	0	0	0
			2091	1312	388	389	2			
1	C	272	Total	C	N	O	S	0	0	0
			2111	1324	391	394	2			
1	D	269	Total	C	N	O	S	0	0	0
			2087	1310	388	387	2			

- Molecule 2 is 4-(DIAZENYLCARBONYL)PYRIDINE (three-letter code: ISZ) (formula:  $C_6H_5N_3O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	3	1		
2	B	1	Total	C	N	O	0	0
			10	6	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			10	6	3	1		
2	D	1	Total	C	N	O	0	0
			10	6	3	1		

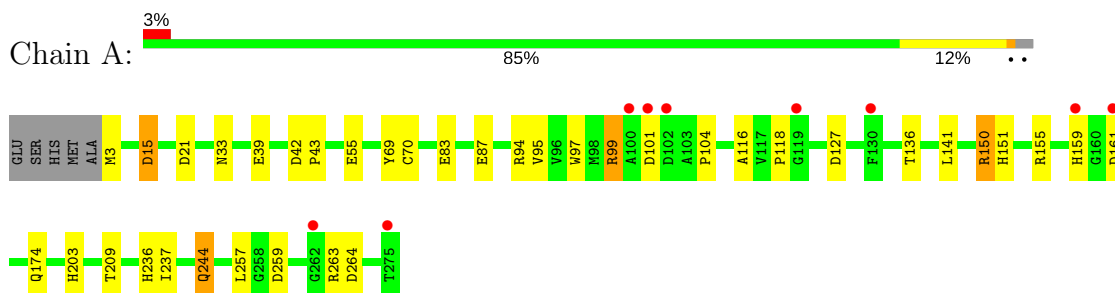
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	248	Total	O	0	0
			248	248		
3	B	196	Total	O	0	0
			196	196		
3	C	173	Total	O	0	0
			173	173		
3	D	101	Total	O	0	0
			101	101		

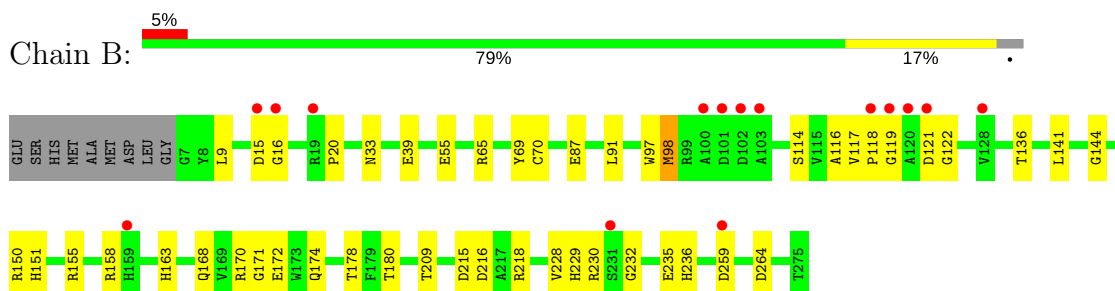
### 3 Residue-property plots [i](#)

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.

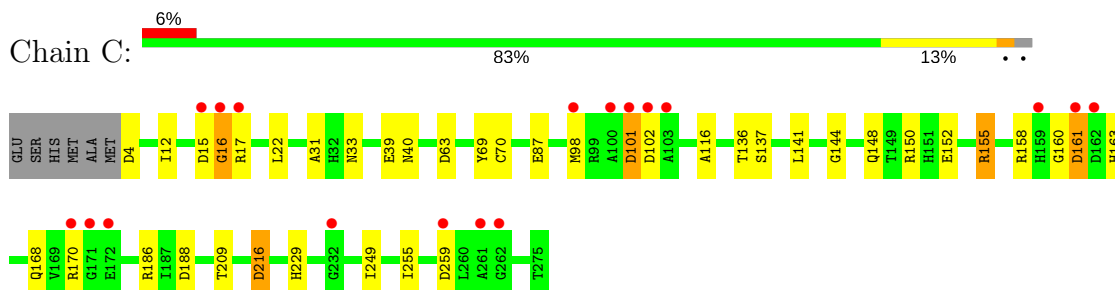
#### • Molecule 1: ARYLAMINE N-ACETYLTRANSFERASE



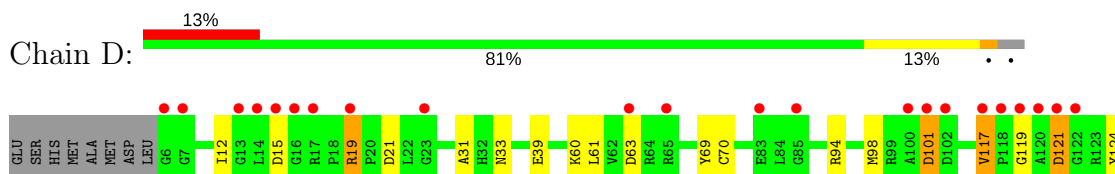
#### • Molecule 1: ARYLAMINE N-ACETYLTRANSFERASE

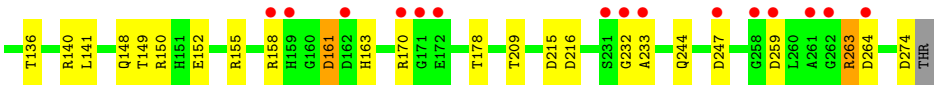


#### • Molecule 1: ARYLAMINE N-ACETYLTRANSFERASE



#### • 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, $\alpha$ , $\beta$ , $\gamma$	101.21Å 106.04Å 140.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.52 – 2.10 28.20 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.4 (84.52-2.10) 92.0 (28.20-2.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.180 , 0.219 0.193 , 0.227	Depositor DCC
$R_{free}$ test set	4104 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9166	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: ISZ

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	0.97	1/2167 (0.0%)	1.02	10/2952 (0.3%)
1	B	0.95	1/2139 (0.0%)	1.01	8/2915 (0.3%)
1	C	0.92	0/2159	0.94	6/2942 (0.2%)
1	D	0.80	0/2135	0.94	10/2910 (0.3%)
All	All	0.91	2/8600 (0.0%)	0.98	34/11719 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	GLU	CG-CD	5.95	1.60	1.51
1	B	55	GLU	CG-CD	5.19	1.59	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	B	170	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	B	259	ASP	CB-CG-OD2	6.92	124.53	118.30
1	B	215	ASP	CB-CG-OD2	6.65	124.28	118.30
1	D	63	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	121	ASP	CB-CG-OD2	6.46	124.11	118.30
1	D	215	ASP	CB-CG-OD2	6.41	124.07	118.30
1	B	170	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	B	218	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	C	259	ASP	CB-CG-OD2	6.21	123.89	118.30
1	D	101	ASP	CB-CG-OD2	6.21	123.89	118.30
1	C	4	ASP	CB-CG-OD2	5.95	123.66	118.30
1	D	247	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	274	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	230	ARG	O-C-N	-5.60	113.73	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	161	ASP	CB-CG-OD2	5.56	123.31	118.30
1	C	216	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	99	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	C	63	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	127	ASP	CB-CG-OD2	5.36	123.13	118.30
1	C	188	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	15	ASP	N-CA-C	5.31	125.35	111.00
1	D	94	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	94	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	15	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	150	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	264	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	155	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	D	121	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	216	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	150	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	21	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	263	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	C	155	ARG	NE-CZ-NH1	5.03	122.81	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	2119	0	2075	37	0
1	B	2091	0	2048	44	0
1	C	2111	0	2066	32	0
1	D	2087	0	2044	22	0
2	A	10	0	5	5	0
2	B	10	0	5	3	0
2	C	10	0	5	3	0
2	D	10	0	5	1	0
3	A	248	0	0	20	0
3	B	196	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	173	0	0	14	0
3	D	101	0	0	8	0
All	All	9166	0	8253	133	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 8.

All (133) 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:B:209:THR:HB	3:B:2152:HOH:O	1.36	1.23
1:C:209:THR:HB	3:C:2028:HOH:O	1.44	1.16
1:B:98:MET:HA	1:B:98:MET:HE3	1.33	1.09
1:A:161:ASP:CG	3:A:2161:HOH:O	1.91	1.06
1:B:98:MET:HA	1:B:98:MET:CE	1.88	1.03
1:B:216:ASP:HB2	3:B:2154:HOH:O	1.63	0.98
1:C:70:CYS:SG	2:C:1276:ISZ:N3	2.37	0.97
1:B:171:GLY:C	3:B:2122:HOH:O	1.99	0.97
1:B:9:LEU:HD13	1:B:16:GLY:O	1.63	0.97
1:C:168:GLN:OE1	3:C:2115:HOH:O	1.83	0.96
1:C:148:GLN:HB2	3:C:2099:HOH:O	1.65	0.95
1:B:70:CYS:HG	2:B:1276:ISZ:HN1	1.12	0.93
1:B:163:HIS:CD2	3:B:2129:HOH:O	2.23	0.91
1:C:161:ASP:O	1:C:163:HIS:HD2	1.53	0.91
1:A:70:CYS:HG	2:A:1276:ISZ:HN1	1.02	0.91
1:B:70:CYS:SG	2:B:1276:ISZ:N3	2.45	0.89
1:A:15:ASP:HB2	3:A:2017:HOH:O	1.72	0.89
1:A:70:CYS:SG	2:A:1276:ISZ:N3	2.47	0.88
1:B:33:ASN:HD21	1:B:136:THR:HA	1.38	0.88
1:B:229:HIS:HD2	3:B:2167:HOH:O	1.57	0.87
1:C:168:GLN:CD	3:C:2115:HOH:O	2.15	0.85
1:B:229:HIS:CD2	3:B:2167:HOH:O	2.31	0.84
1:D:264:ASP:HB2	3:D:2096:HOH:O	1.77	0.84
1:B:33:ASN:HD22	1:B:150:ARG:HH21	1.25	0.82
1:A:259:ASP:HB2	3:A:2068:HOH:O	1.80	0.81
1:C:161:ASP:O	1:C:163:HIS:CD2	2.34	0.80
1:A:161:ASP:CB	3:A:2161:HOH:O	2.27	0.77
1:B:172:GLU:N	3:B:2122:HOH:O	2.16	0.76
1:D:121:ASP:HA	3:D:2038:HOH:O	1.84	0.76
1:B:163:HIS:HD2	3:B:2129:HOH:O	1.65	0.76
1:D:33:ASN:HD22	1:D:150:ARG:HH21	1.32	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ASN:HD21	1:C:136:THR:HA	1.52	0.75
1:B:180:THR:HA	3:B:2129:HOH:O	1.88	0.74
1:C:70:CYS:HG	2:C:1276:ISZ:HN1	1.17	0.73
1:A:237:ILE:HG12	1:B:235:GLU:HG3	1.72	0.72
1:C:33:ASN:HD22	1:C:150:ARG:HH21	1.37	0.72
1:A:161:ASP:HB3	3:A:2161:HOH:O	1.87	0.70
1:A:159:HIS:CG	3:A:2159:HOH:O	2.47	0.68
1:B:117:VAL:C	3:B:2081:HOH:O	2.32	0.68
1:D:33:ASN:HD21	1:D:136:THR:HA	1.59	0.67
1:B:98:MET:CA	1:B:98:MET:HE3	2.21	0.67
1:C:161:ASP:N	3:C:2111:HOH:O	2.25	0.66
1:C:152:GLU:HB2	3:C:2103:HOH:O	1.94	0.66
1:D:244:GLN:HG3	3:D:2090:HOH:O	1.96	0.66
1:A:236:HIS:CD2	3:A:2216:HOH:O	2.49	0.65
1:D:70:CYS:SG	2:D:1276:ISZ:N3	2.66	0.64
1:A:33:ASN:HD21	1:A:136:THR:HA	1.63	0.63
1:C:102:ASP:HB2	3:C:2069:HOH:O	1.99	0.62
1:A:33:ASN:HD22	1:A:150:ARG:HH21	1.48	0.61
1:A:203:HIS:HE1	3:A:2194:HOH:O	1.83	0.61
1:A:174:GLN:HG2	3:A:2048:HOH:O	2.02	0.60
1:C:160:GLY:O	1:C:161:ASP:CB	2.49	0.59
1:D:124:TYR:CE2	1:D:140:ARG:HG2	2.38	0.59
1:C:98:MET:HG3	1:C:98:MET:O	2.02	0.58
1:C:33:ASN:HD22	1:C:150:ARG:NH2	2.02	0.56
1:B:98:MET:HE2	1:B:98:MET:HA	1.81	0.56
1:A:70:CYS:SG	2:A:1276:ISZ:N2	2.78	0.56
1:B:228:VAL:HB	1:B:235:GLU:HB3	1.87	0.56
1:A:33:ASN:HD22	1:A:150:ARG:NH2	2.04	0.55
1:B:144:GLY:O	1:B:155:ARG:NH1	2.38	0.55
1:D:12:ILE:HD12	1:D:31:ALA:HB3	1.88	0.55
1:B:171:GLY:CA	3:B:2122:HOH:O	2.47	0.55
1:A:15:ASP:HB2	3:A:2018:HOH:O	2.06	0.55
1:A:136:THR:OG1	1:A:151:HIS:HD2	1.91	0.54
1:B:98:MET:CA	1:B:98:MET:CE	2.68	0.54
1:A:118:PRO:HA	3:A:2118:HOH:O	2.07	0.54
1:A:42:ASP:HB2	1:A:43:PRO:HD3	1.89	0.54
1:B:9:LEU:CD1	1:B:16:GLY:O	2.48	0.54
1:B:209:THR:HG23	3:B:2161:HOH:O	2.06	0.54
1:D:263:ARG:HG2	1:D:263:ARG:HH11	1.73	0.54
1:C:70:CYS:SG	2:C:1276:ISZ:N2	2.81	0.54
1:D:33:ASN:HD22	1:D:150:ARG:NH2	2.03	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ASP:O	1:C:102:ASP:HB2	2.08	0.53
1:A:203:HIS:HD2	3:A:2075:HOH:O	1.90	0.53
1:A:99:ARG:NH1	1:A:104:PRO:O	2.43	0.51
1:C:216:ASP:HB2	3:C:2139:HOH:O	2.10	0.51
1:C:15:ASP:C	1:C:16:GLY:O	2.49	0.51
1:A:159:HIS:CE1	3:A:2159:HOH:O	2.63	0.51
1:A:159:HIS:CD2	3:A:2159:HOH:O	2.63	0.50
1:D:12:ILE:O	1:D:31:ALA:HB1	2.11	0.50
1:B:20:PRO:HD3	3:B:2056:HOH:O	2.11	0.50
1:D:233:ALA:N	3:D:2084:HOH:O	2.45	0.50
1:A:15:ASP:CB	3:A:2018:HOH:O	2.59	0.50
1:C:186:ARG:HD3	3:C:2122:HOH:O	2.11	0.50
1:D:60:LYS:HG2	1:D:61:LEU:HD12	1.93	0.50
1:C:144:GLY:O	1:C:155:ARG:HD2	2.12	0.50
1:C:148:GLN:OE1	3:C:2099:HOH:O	2.19	0.49
1:D:19:ARG:HB2	3:D:2003:HOH:O	2.12	0.49
1:B:70:CYS:SG	2:B:1276:ISZ:N2	2.86	0.49
1:B:168:GLN:HG2	1:B:171:GLY:O	2.13	0.49
1:B:33:ASN:HD22	1:B:150:ARG:NH2	2.03	0.49
1:A:244:GLN:H	1:A:244:GLN:NE2	2.11	0.48
1:C:249:ILE:HG23	1:C:255:ILE:HD12	1.94	0.48
1:D:98:MET:HG2	3:D:2029:HOH:O	2.13	0.48
1:B:118:PRO:N	3:B:2081:HOH:O	2.47	0.48
1:C:158:ARG:NE	3:C:2111:HOH:O	2.44	0.48
3:C:2148:HOH:O	1:D:244:GLN:HG2	2.13	0.47
1:A:87:GLU:HB3	1:A:116:ALA:HB3	1.96	0.47
1:C:148:GLN:HG2	3:C:2100:HOH:O	2.14	0.47
1:A:3:MET:HE2	1:A:83:GLU:HG2	1.97	0.47
1:D:149:THR:OG1	1:D:152:GLU:O	2.27	0.47
1:B:172:GLU:HA	3:B:2122:HOH:O	2.14	0.47
1:D:209:THR:HG23	3:D:2077:HOH:O	2.15	0.46
1:A:161:ASP:OD2	3:A:2161:HOH:O	2.18	0.46
3:A:2218:HOH:O	1:B:236:HIS:CD2	2.68	0.46
1:C:160:GLY:O	1:C:161:ASP:HB2	2.16	0.46
1:B:87:GLU:HB3	1:B:116:ALA:HB3	1.97	0.45
1:C:12:ILE:O	1:C:31:ALA:HB1	2.16	0.45
1:C:40:ASN:CG	3:C:2028:HOH:O	2.54	0.45
1:B:122:GLY:HA2	3:B:2086:HOH:O	2.16	0.45
1:A:244:GLN:HG2	1:B:232:GLY:HA3	1.99	0.44
1:D:21:ASP:HA	1:D:117:VAL:CG1	2.47	0.44
1:A:150:ARG:HD2	3:A:2148:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:GLN:CG	3:B:2123:HOH:O	2.66	0.43
1:A:95:VAL:HG21	2:A:1276:ISZ:C5	2.48	0.43
1:A:257:LEU:C	1:A:259:ASP:N	2.72	0.43
1:A:209:THR:HG23	3:A:2206:HOH:O	2.17	0.43
1:B:119:GLY:O	3:B:2083:HOH:O	2.22	0.43
1:C:15:ASP:O	1:C:16:GLY:O	2.36	0.43
1:C:229:HIS:CD2	1:C:229:HIS:N	2.86	0.43
1:A:97:TRP:HZ3	3:A:2060:HOH:O	2.01	0.43
1:A:42:ASP:CB	1:A:43:PRO:HD3	2.49	0.42
1:D:163:HIS:O	1:D:178:THR:HA	2.19	0.42
1:B:33:ASN:HD21	1:B:136:THR:CA	2.19	0.42
1:B:91:LEU:HD11	1:B:114:SER:HB2	2.01	0.42
1:D:161:ASP:O	1:D:163:HIS:HD2	2.02	0.42
1:B:163:HIS:O	1:B:178:THR:HA	2.19	0.42
1:B:136:THR:OG1	1:B:151:HIS:HD2	2.03	0.42
1:D:232:GLY:C	3:D:2084:HOH:O	2.58	0.41
1:C:87:GLU:HB3	1:C:116:ALA:HB3	2.02	0.41
1:A:95:VAL:HG21	2:A:1276:ISZ:H5	2.02	0.40
1:B:172:GLU:CA	3:B:2122:HOH:O	2.64	0.40
1:B:97:TRP:CD1	1:B:98:MET:HG2	2.56	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	271/278 (98%)	263 (97%)	8 (3%)	0	100	100
1	B	267/278 (96%)	260 (97%)	7 (3%)	0	100	100
1	C	270/278 (97%)	261 (97%)	7 (3%)	2 (1%)	24	19
1	D	267/278 (96%)	255 (96%)	11 (4%)	1 (0%)	36	34
All	All	1075/1112 (97%)	1039 (97%)	33 (3%)	3 (0%)	43	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	161	ASP
1	D	119	GLY
1	C	16	GLY

### 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	220/224 (98%)	214 (97%)	6 (3%)	48	51
1	B	217/224 (97%)	210 (97%)	7 (3%)	42	44
1	C	219/224 (98%)	211 (96%)	8 (4%)	37	38
1	D	216/224 (96%)	204 (94%)	12 (6%)	23	20
All	All	872/896 (97%)	839 (96%)	33 (4%)	36	36

All (33) 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	101	ASP
1	A	141	LEU
1	A	244	GLN
1	B	39	GLU
1	B	65	ARG
1	B	69	TYR
1	B	98	MET
1	B	141	LEU
1	B	158	ARG
1	B	264	ASP
1	C	17	ARG
1	C	22	LEU
1	C	39	GLU
1	C	69	TYR

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Mol	Chain	Res	Type
1	C	101	ASP
1	C	137	SER
1	C	141	LEU
1	C	170	ARG
1	D	19	ARG
1	D	39	GLU
1	D	69	TYR
1	D	101	ASP
1	D	117	VAL
1	D	141	LEU
1	D	148	GLN
1	D	155	ARG
1	D	158	ARG
1	D	170	ARG
1	D	259	ASP
1	D	263	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	108	GLN
1	A	151	HIS
1	A	168	GLN
1	A	203	HIS
1	A	244	GLN
1	B	33	ASN
1	B	148	GLN
1	B	151	HIS
1	B	159	HIS
1	B	244	GLN
1	C	33	ASN
1	C	108	GLN
1	C	151	HIS
1	C	163	HIS
1	C	229	HIS
1	D	33	ASN
1	D	108	GLN
1	D	151	HIS
1	D	163	HIS
1	D	168	GLN
1	D	244	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 ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	ISZ	A	1276	-	9,10,10	1.74	1 (11%)	12,12,12	1.36	2 (16%)
2	ISZ	B	1276	-	9,10,10	1.11	1 (11%)	12,12,12	1.60	3 (25%)
2	ISZ	C	1276	-	9,10,10	1.00	1 (11%)	12,12,12	1.17	1 (8%)
2	ISZ	D	1276	-	9,10,10	1.94	1 (11%)	12,12,12	1.16	1 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ISZ	A	1276	-	-	0/4/6/6	0/1/1/1
2	ISZ	B	1276	-	-	0/4/6/6	0/1/1/1
2	ISZ	C	1276	-	-	0/4/6/6	0/1/1/1
2	ISZ	D	1276	-	-	0/4/6/6	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1276	ISZ	C1-C6	2.60	1.53	1.49
2	B	1276	ISZ	C1-C6	2.72	1.53	1.49
2	A	1276	ISZ	C1-C6	4.69	1.56	1.49
2	D	1276	ISZ	C1-C6	5.22	1.56	1.49

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1276	ISZ	C3-C5-N1	-2.58	119.12	123.62
2	B	1276	ISZ	C2-C4-N1	-2.17	119.85	123.62
2	D	1276	ISZ	C5-N1-C4	2.09	121.86	116.84
2	C	1276	ISZ	C5-N1-C4	2.18	122.08	116.84
2	A	1276	ISZ	C5-N1-C4	2.50	122.86	116.84
2	B	1276	ISZ	C5-N1-C4	2.56	123.00	116.84
2	B	1276	ISZ	C1-C6-N2	2.63	118.97	114.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1276	ISZ	5	0
2	B	1276	ISZ	3	0
2	C	1276	ISZ	3	0
2	D	1276	ISZ	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	273/278 (98%)	-0.02	9 (3%) 46 54	8, 16, 34, 52	0
1	B	269/278 (96%)	0.17	15 (5%) 24 30	10, 21, 42, 55	0
1	C	272/278 (97%)	0.29	18 (6%) 18 23	12, 23, 45, 58	0
1	D	269/278 (96%)	0.79	37 (13%) 3 4	16, 34, 59, 73	0
All	All	1083/1112 (97%)	0.31	79 (7%) 15 19	8, 23, 50, 73	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	ASP	7.4
1	D	121	ASP	7.3
1	B	101	ASP	7.1
1	D	102	ASP	6.5
1	B	119	GLY	6.3
1	D	232	GLY	6.2
1	B	120	ALA	5.8
1	A	101	ASP	5.7
1	C	102	ASP	5.6
1	C	16	GLY	5.6
1	D	262	GLY	5.6
1	D	120	ALA	5.4
1	C	101	ASP	5.3
1	B	16	GLY	5.2
1	D	119	GLY	5.1
1	D	101	ASP	5.0
1	B	102	ASP	5.0
1	D	17	ARG	4.6
1	D	15	ASP	4.6
1	B	121	ASP	4.6
1	D	118	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	16	GLY	4.6
1	C	161	ASP	4.6
1	A	102	ASP	4.3
1	D	259	ASP	4.2
1	C	98	MET	4.1
1	C	262	GLY	4.0
1	C	100	ALA	3.9
1	D	159	HIS	3.9
1	B	159	HIS	3.7
1	A	161	ASP	3.7
1	D	6	GLY	3.6
1	D	170	ARG	3.4
1	D	172	GLU	3.4
1	C	171	GLY	3.4
1	C	17	ARG	3.4
1	D	19	ARG	3.3
1	C	15	ASP	3.3
1	D	258	GLY	3.3
1	C	261	ALA	3.3
1	B	100	ALA	3.3
1	B	118	PRO	3.2
1	D	100	ALA	3.2
1	D	14	LEU	3.1
1	C	159	HIS	3.0
1	D	231	SER	3.0
1	D	13	GLY	3.0
1	A	262	GLY	2.8
1	D	7	GLY	2.7
1	B	231	SER	2.7
1	C	172	GLU	2.7
1	D	233	ALA	2.7
1	C	162	ASP	2.6
1	C	232	GLY	2.6
1	C	170	ARG	2.5
1	D	171	GLY	2.5
1	D	117	VAL	2.4
1	D	158	ARG	2.4
1	A	275	THR	2.4
1	A	130	PHE	2.4
1	A	159	HIS	2.4
1	D	83	GLU	2.4
1	B	103	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	122	GLY	2.4
1	D	65	ARG	2.3
1	D	23	GLY	2.3
1	D	162	ASP	2.3
1	A	100	ALA	2.2
1	D	261	ALA	2.2
1	A	119	GLY	2.2
1	C	103	ALA	2.2
1	C	259	ASP	2.2
1	B	128	VAL	2.1
1	B	259	ASP	2.1
1	D	247	ASP	2.1
1	B	19	ARG	2.0
1	D	264	ASP	2.0
1	D	85	GLY	2.0
1	D	63	ASP	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ISZ	D	1276	10/10	0.81	0.28	52,54,55,56	0
2	ISZ	A	1276	10/10	0.87	0.25	36,39,43,43	0
2	ISZ	C	1276	10/10	0.87	0.21	40,43,46,46	0
2	ISZ	B	1276	10/10	0.88	0.20	34,37,41,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.