



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:14 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 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/ValidationPDFNotes.html>

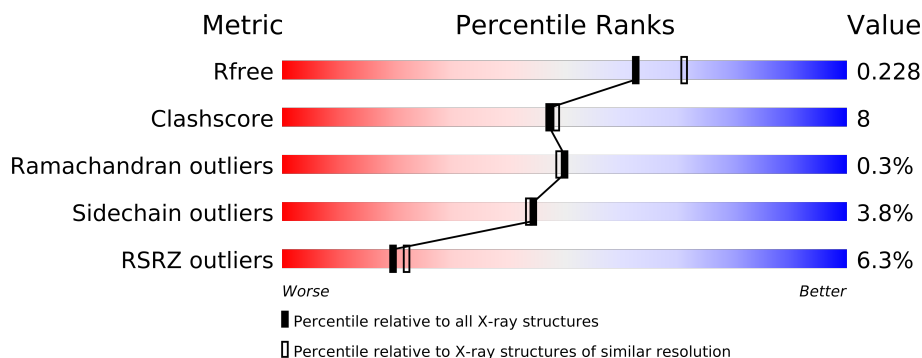
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	278	
1	B	278	
1	C	278	
1	D	278	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ISZ	A	1276	-	X
2	ISZ	B	1276	-	X
2	ISZ	C	1276	-	X
2	ISZ	D	1276	-	X

2 Entry composition i

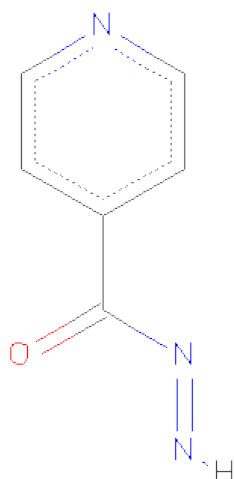
There are 3 unique types of molecules in this entry. The entry contains 9166 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

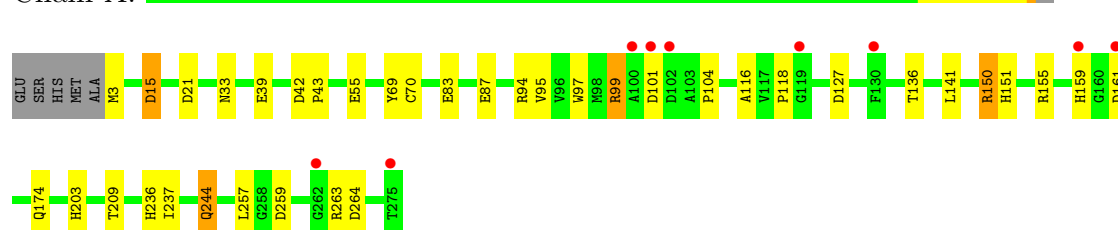
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	248	Total	O	0	0
			248	248		
3	B	196	Total	O	0	0
			196	196		
3	C	173	Total	O	0	0
			173	173		
3	D	101	Total	O	0	0
			101	101		

3 Residue-property plots

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.

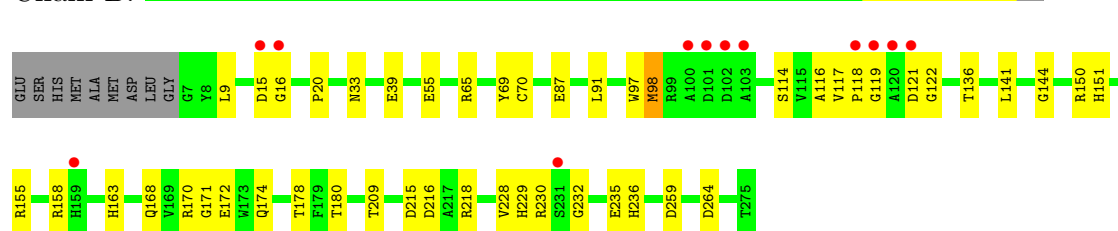
• Molecule 1: ARYLAMINE N-ACETYLTRANSFERASE

Chain A:



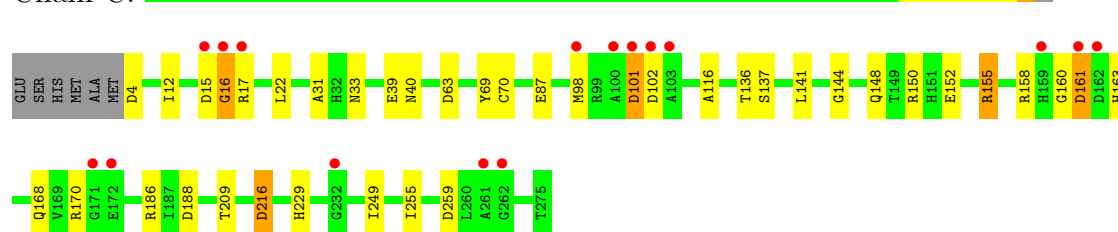
• Molecule 1: ARYLAMINE N-ACETYLTRANSFERASE

Chain B:



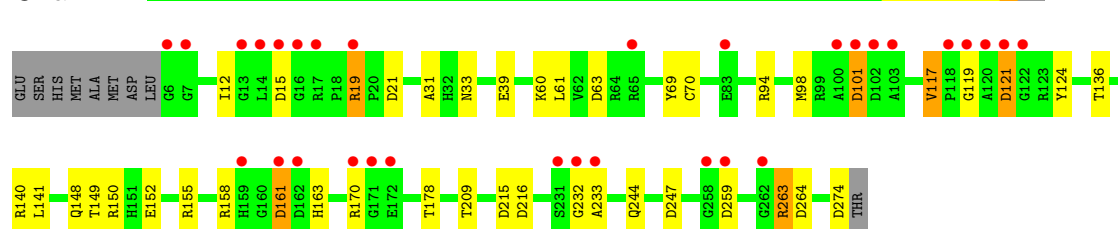
• Molecule 1: ARYLAMINE N-ACETYLTRANSFERASE

Chain C:



• Molecule 1: ARYLAMINE N-ACETYLTRANSFERASE

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.180 , 0.219 0.193 , 0.228	Depositor DCC
R_{free} test set	4104 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 33.8	EDS
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 81906 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9166	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	248	0	0	20	0
3	B	196	0	0	19	0
3	C	173	0	0	14	0
3	D	101	0	0	8	0
All	All	9166	0	8253	133	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (133) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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:B:98:MET:CA	1:B:98:MET:CE	2.68	0.54
1:A:136:THR:OG1	1:A:151:HIS:HD2	1.91	0.54
1:A:118:PRO:HA	3:A:2118:HOH:O	2.07	0.54
1:B:9:LEU:CD1	1:B:16:GLY:O	2.48	0.54
1:A:42:ASP:HB2	1:A:43:PRO:HD3	1.89	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
1:C:101:ASP:O	1:C:102:ASP:HB2	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:168:GLN:HG2	1:B:171:GLY:O	2.13	0.49
1:B:70:CYS:SG	2:B:1276:ISZ:N2	2.86	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:C:158:ARG:NE	3:C:2111:HOH:O	2.44	0.48
1:B:118:PRO:N	3:B:2081:HOH:O	2.47	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:D:149:THR:OG1	1:D:152:GLU:O	2.27	0.47
1:A:3:MET:HE2	1:A:83:GLU:HG2	1.97	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:40:ASN:CG	3:C:2028:HOH:O	2.54	0.45
1:C:12:ILE:O	1:C:31:ALA:HB1	2.16	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:257:LEU:C	1:A:259:ASP:N	2.72	0.43
1:C:15:ASP:O	1:C:16:GLY:O	2.36	0.43
1:B:119:GLY:O	3:B:2083:HOH:O	2.22	0.43
1:A:209:THR:HG23	3:A:2206:HOH:O	2.17	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:B:172:GLU:CA	3:B:2122:HOH:O	2.64	0.40
1:A:95:VAL:HG21	2:A:1276:ISZ:H5	2.02	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

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	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%)	30	23
1	D	267/278 (96%)	255 (96%)	11 (4%)	1 (0%)	43	39
All	All	1075/1112 (97%)	1039 (97%)	33 (3%)	3 (0%)	50	49

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 ⓘ

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%)	57	60
1	B	217/224 (97%)	210 (97%)	7 (3%)	51	52
1	C	219/224 (98%)	211 (96%)	8 (4%)	45	45
1	D	216/224 (96%)	204 (94%)	12 (6%)	30	25
All	All	872/896 (97%)	839 (96%)	33 (4%)	44	44

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
1	C	101	ASP
1	C	137	SER
1	C	141	LEU

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Mol	Chain	Res	Type
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 chains 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	1.71	1 (11%)	12,12,12	1.53	3 (25%)
2	ISZ	B	1276	-	9,10,10	1.09	1 (11%)	12,12,12	1.91	3 (25%)
2	ISZ	C	1276	-	9,10,10	0.98	1 (11%)	12,12,12	1.30	2 (16%)
2	ISZ	D	1276	-	9,10,10	1.90	1 (11%)	12,12,12	1.40	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	D	1276	ISZ	C1-C6	5.09	1.56	1.49
2	A	1276	ISZ	C1-C6	4.58	1.56	1.49
2	B	1276	ISZ	C1-C6	2.67	1.53	1.49
2	C	1276	ISZ	C1-C6	2.56	1.53	1.49

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1276	ISZ	C1-C6-N2	4.51	118.97	113.06
2	D	1276	ISZ	C1-C6-N2	3.43	117.56	113.06
2	A	1276	ISZ	C1-C6-N2	3.18	117.23	113.06
2	A	1276	ISZ	C3-C5-N1	-2.49	119.12	123.63
2	C	1276	ISZ	C1-C6-N2	2.46	116.28	113.06
2	B	1276	ISZ	C5-N1-C4	2.42	123.00	116.84
2	A	1276	ISZ	C5-N1-C4	2.37	122.86	116.84
2	B	1276	ISZ	C2-C4-N1	-2.09	119.85	123.63
2	C	1276	ISZ	C5-N1-C4	2.06	122.08	116.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	273/278 (98%)	-0.09	9 (3%) 44 49	8, 16, 34, 52	0
1	B	269/278 (96%)	0.10	12 (4%) 32 35	10, 21, 42, 55	0
1	C	272/278 (97%)	0.21	16 (5%) 22 24	12, 23, 45, 58	0
1	D	269/278 (96%)	0.68	31 (11%) 5 6	16, 34, 59, 73	0
All	All	1083/1112 (97%)	0.22	68 (6%) 19 22	8, 23, 50, 73	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	GLY	6.7
1	B	15	ASP	6.5
1	D	121	ASP	6.5
1	D	102	ASP	6.0
1	B	101	ASP	5.9
1	C	102	ASP	5.3
1	C	101	ASP	5.3
1	D	232	GLY	5.0
1	D	120	ALA	5.0
1	C	16	GLY	5.0
1	A	101	ASP	5.0
1	B	102	ASP	5.0
1	D	262	GLY	4.9
1	B	120	ALA	4.9
1	D	16	GLY	4.8
1	D	119	GLY	4.6
1	B	16	GLY	4.5
1	D	101	ASP	4.3
1	D	17	ARG	4.2
1	C	161	ASP	4.2
1	D	15	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	118	PRO	4.0
1	D	259	ASP	4.0
1	B	121	ASP	3.9
1	D	159	HIS	3.9
1	A	102	ASP	3.7
1	C	100	ALA	3.7
1	C	98	MET	3.4
1	D	100	ALA	3.4
1	B	159	HIS	3.3
1	A	161	ASP	3.3
1	C	262	GLY	3.2
1	C	17	ARG	3.2
1	D	6	GLY	3.2
1	D	14	LEU	3.2
1	D	13	GLY	3.1
1	D	172	GLU	3.1
1	C	15	ASP	2.9
1	B	100	ALA	2.9
1	C	171	GLY	2.8
1	D	19	ARG	2.8
1	C	261	ALA	2.8
1	C	159	HIS	2.8
1	D	233	ALA	2.7
1	D	258	GLY	2.7
1	B	118	PRO	2.7
1	C	232	GLY	2.6
1	D	171	GLY	2.6
1	D	170	ARG	2.6
1	D	231	SER	2.5
1	B	103	ALA	2.5
1	C	172	GLU	2.5
1	D	7	GLY	2.5
1	B	231	SER	2.4
1	A	100	ALA	2.3
1	C	162	ASP	2.3
1	C	103	ALA	2.3
1	D	83	GLU	2.2
1	D	122	GLY	2.2
1	D	162	ASP	2.2
1	A	262	GLY	2.2
1	A	159	HIS	2.1
1	A	275	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	130	PHE	2.1
1	D	161	ASP	2.1
1	D	103	ALA	2.0
1	D	65	ARG	2.0
1	A	119	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ISZ	D	1276	10/10	0.27	3.31	52,54,55,56	0
2	ISZ	A	1276	10/10	0.24	2.34	36,39,43,43	0
2	ISZ	B	1276	10/10	0.18	2.32	34,37,41,42	0
2	ISZ	C	1276	10/10	0.19	2.25	40,43,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.